DEVELOPING A PROPER NANO MATERIAL TO USE IN CUISINE CLAY POTTERY

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Master of Science (Major Component of Research)

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Thesis/Dissertation submitted in partial fulfillment of the requirements for the degree

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DECLARATION

I declare that this is my own work and this thesis/dissertation does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any other University or Institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text. I retain the right to use this content in whole or part in future works (such as articles or books).

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The above candidate has carried out research for the PhD/MPhil/Masters thesis/dissertation under my supervision. I confirm that the declaration made above by the student is true and correct.

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DEDICATION

This thesis is dedicated to all those who provided unwavering support and encouragement throughout my academic journey. It stands not merely as a scholarly document, but as a testament to the perseverance and dedication applied during one of the most difficult periods of my life. This accomplishment is not solely my own, it is equally a reflection of the compassion, guidance, and solidarity extended by the remarkable individuals who stood by me during this transformative academic endeavor.

This is dedicated to my lovely family for the continuous encouragement towards these achievements. Especially to my loving husband for supporting me in maintaining my morale, for continuing this effort until success and for my parents for the immense support and the consideration given me within this period. Specially I should mention, this is dedicated as a tribute to my late farther who was passed away during this academic period as fulfilling one of his dreams regarding my academic path.

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To my friends and research colleagues, I dedicate this for their inspiration for fulfilling this research positively and successfully.

Finally, I dedicate this thesis for anyone who is interested in research, to courageous people to continue their academic studies effectively and efficiently and to all individuals who support me to be independent in my academic path and my personal life.

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ABSTRACT

Clay pottery, originating at dawn in civilization, is a fundamental village industry primarily used as eco-friendly and health safe cookware. Currently, nonstick metal cookware is popular for convenience but poses health risks from toxic compound releasing to food. Despite its traditional use, clay cookware tends to stick food to the inner surface of pottery during cooking, limiting its functionality. Thus, this study aims to develop a proper mineral nano material to improve the nonstick properties of clay cookware, addressing a key industrial gap. Sri Lankan industrial clays, minerals and their physiochemical properties were identified through the primary data and secondary data from an industrial survey and literature review. Using Gaussian Software under computational chemistry, suitable mineral type was identified through molecular modeling and binding energy calculation to combine with the most common clay. The nonstick performance of clay and mineral combination was assessed via binding energy analysis with fat/oil molecules. Red clay is the most used material for cooking pottery, predominantly utilized by small-scale domestic manufacturers. This sector surpasses medium-scale and government supporting units in usage. Male participation is highest compared to female and both gender involvement. BE calculations show Red clay and Apatite combination has the highest stability with the highest negative BE –3177 kcal/mol. Red clay with fats/oils mixtures have negative BEs of –1552, –2142, –2117, and –1522 kcal/mol, indicating strong interactions, while the Red clay and Apatite mixture shows the positive BEs of 3212, 2376, 2450, and 3903 kcal/mol with fat/oils indicating weaker interactions with less stable systems. The Red clay and Apatite blend reduces fat/oil adhesion and enhances nonstick properties by making Apatite is the ideal mineral to collaborate with Red clay to make pottery. When considering the applying of nanotechnology, using nanoscale particles increases binding energy making the Red clay and Apatite system more stable and nonstick.

Keywords: Nonstick Cooking Pottery, Clay and Mineral, Computational Chemistry, Binding Energy, Nanotechnology

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LIST OF ABBREVIATIONS

Abbreviation	Description
BE	Binding Energy
GS	Gaussian Software
AU	Atomic Unit
PTFE	Teflon, Poly Tetra Fluoro Ethylene
PFC	Poly Fluoro Carbon
IARC	The International Agency for Research on Cancer
PFOA	Perfluorooctanoic acid
kcal/mol	kilocalorie per mole
ICP device	Inductively Coupled Plasma device
PFOA	Perfluorooctanoic acid
PFOS	Perfluoro Octane Sulfonate
PFAS	Per- and polyfluoroalkyl substances
HFPO	Hexafluoropropylene oxide
PFBS	Perfluorobutane Sulfonic acid
EPA	United States Environmental Protection Agency
GDP	Gross Domestic Product
NMR spectra	Nuclear magnetic resonance spectra
CD spectra	Circular Dichroism spectra
IR spectra	Infrared spectra
DFT	Density Functional Theory
MD	Molecular Dynamics
MM	Molecular Mechanics
GNM	Gaussian Network Model
PBC	Periodic Boundary Conditions
E	Energy
Opt + Freq	Geometry optimization and Frequency calculation

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CHAPTER 1

INTRODUCTION

1.1 Background of The Study

Along with the emergence of civilization the clay pottery industry has an immemorial antiquity as a basic village industry. Mostly these clay potteries are used as cookware and there are advantages in using them for cuisine purposes as clay is an environmentally friendly and eco-friendly material with minimum harm to the environment. Other special characteristics of clay pottery are antibacterial properties, consisting of natural minerals, non-flammable, resistant to heat, mould and rusts and it has artistic and functional value (Amboro et al., 2023). With the increased use of clay potteries for cooking purpose, the advancements are required by consumers for the user-friendly purpose due to it should prevent the food stickiness, easy to wash and clean, resistance to scratch, cost effective ,even distribution of heat and save on fuel ,reduces the cooking time, cooks tasty meals without using oil or with less oil, suitable to modern kitchens and satisfy the new generation than the existing clay potteries (Ruengcharungpong et al., 2019).

Various types of materials are used to manufacture cookware, and they are different types of metal materials, plastics, Teflon (PTFE), clay, stones and glass (Shamloo et al., 2023). Metals are the widely used material type to produce cookware and utensils for cuisine purposes among the above materials and aluminum, iron, stainless steel, silver, brass, gold and copper are some of the metal constituents used for preparing those cuisine utensils. Anodized or non-anodized metal cookware are consumed for cuisine purposes and however, this is not a long-term solution, as over time the anodized or coated layers are scratched due to abrasion, potentially leading to food contamination and various health issues (Alabi and Adeoluwa, 2020).

Non-stick metal cookware are very popular kitchen utensils in the current society due to their user-friendliness. Currently Poly Tetra Fluoro Ethylene (PTFE) and Poly Fluoro Carbon (PFC) are the widely used non-stick coating materials, and they are coated in the inner surface of the metal vessels as a layer (Ismaeili et al., 2022). These artificial (Coyle, 2023) polymers are notable for their non-stick properties, strong mechanical performance and low flammability (Ismaeili et al., 2022). However, their poor resistance to abrasion and heat are major harmful properties of these polymers (Hatzikiriakos, 2012). The International Agency for Research on Cancer (IARC) has been identified these nonstick chemicals PTFE and PFOA as “possibly carcinogenic to humans.” (Bansal et al., 2020).

Sri Lanka is a country enriched with countless natural treasures by creating a home for a wide range of clay mineral types. These raw clay materials are classified based on their role in producing different kinds of clayware. There are three main clay mineral types called Earthenware clay (Red Clay), Ball clay and White clay, each found in different regions. Cleaner layers of these clay types are used in production of pottery, porcelain and ceramic items (Export Development Board Sri Lanka, 2021). In addition to that, kaolinite, Montmorillonite, Illite, gibbsite, hydroxy-interlayered vermiculite, boehmite, vermiculite, mica and other types are the other clay mineral types in Sri Lanka (Export Development Board Sri Lanka, 2020). Sri Lanka is rich in non-metallic mineral resources. According to studies done by the Geological Survey and Mines Bureau, the country's mineral wealth is mainly made up of industrial minerals. They are Graphite, Silica Sand, Quartz, Feldspar, Apatite (Phosphate Rock), Mica, Ilmenite, Rutile, Zircon, Garnet Sand, Calcite and Dolomite (Weerakoon, 2013).

Concerning these matters regarding existing clay potteries and metal cookware, there is a requirement for clay potteries with advanced improved properties due to the existing felicitated features of clay for human consumption than metal cookware. This research is focused on identifying a proper mineral material to collaborate with clay during pottery making to enhance the nonstick property of clay cooking pottery. It leads to prevention of food stickiness to the inner surface of the vessel and for using the property improved clay pottery as a replacement for nonstick metal cookware. Computational Chemistry is used to identify the appropriate mineral type based on the Binding Energies of each clay mineral type. The importance of using nanotechnology for making nano material of minerals is discussed in the study. Fat content in the food has been identified as a predominant factor that affects food stickiness and nonstick property of identified clay mineral collaboration is tested by using the fat content.

Developing proper nano material from minerals, to use in cooking clay potteries is an important identification due to the value addition to the clay potteries and mineral type by converting the clay potteries to user friendly items and preventing health disorders occurred through metal nonstick vessels consumption.

1.2 Research Gap Identification

Currently the use of metal cooking vessels is very popular due to their user friendliness. Metal cookware are produced as nonstick, anodized or non-anodized vessels (Alabi and Adeoluwa, 2020). Even though non-stick vessels are the most widespread item, using the metal cookware cause hygienic problems in human beings. The removal of the inside coating on the inner surface of the metal pot and then it destroys the quality of the food. Therefore, bad health conditions occur in humans including metal and polymer fume fever and Fatal acute pulmonary oedema diseases (Ismaeili et al., 2022; Hatzikiriakos, 2012; Lee et al., 1997; Greenberg & Vearrier, 2015).

Clay has important favorable characteristics to use in cuisine purposes and due to that reason, it has been used to make clay pottery since ancient times (Amboro et al., 2023). Even though clay cooking pottery plays a major role in the domestic cooking sector, people meet with inconveniences of the clay pottery during the cooking. Food stickiness to the inner surface of the clay pottery and cleaning issues have been identified as disturbances in using them. The seasoning should be done before using for cooking to avoid the sticking and these facts are reasons to reduce the user-friendliness of clay cooking pottery.

Therefore, there is a need for an advanced cooking vessel to avoid the above-mentioned issues with improved properties and as suitable for modern kitchen with user friendliness. Hence, proper material selection is the essential thing to ensure the advancements of the cooking vessels. Though clay is a proper material as a replacement for metals due to its favorable characteristics, nonstick and other user-friendly properties similar to metal vessels need to be improved. Thus, the identification and development of proper material which can be improved the nonstick property to collaborate with clay is essential to make advanced clay pottery. As Sri Lanka is enriched with several natural minerals the attention is given to develop the material from minerals instead of using artificial non-stick materials.

1.3 Aims and Objectives

This study aims to develop a proper nano mineral material to collaborate with clay in making cooking clay pottery. Main objectives of this research are.

1. To identify the industrial need of developing proper nano material to use in clay pottery which is used for cuisine purposes.
2. To identify the proper material which can be used as a nanomaterial for clay pottery.
3. To analyze the performances of the identified clay and mineral combination for nano composite.

1.4 Methodology

This study was aligned under four major steps.

1. Collecting Primary and Secondary Data.
2. Find out the physical and chemical properties of each clay type and clay minerals.
3. Identify a suitable mineral nano material to apply for clay pottery.
4. Analyze the nonstick performances of the identified clay and mineral combination.

The primary data collection was done through the industrial survey in the clay pottery industry. Initially the Gampaha District was selected for field visits to find out the main clay type, which is used in the cooking clay pottery industry, the industry type, the gender involvement, major types of cuisine clay potteries and non-cuisine clay potteries and steps of making cuisine clay potteries.

The secondary data collection was done through the literature survey to find out the main clay types to use in the clay pottery industry and to identify the abundant clay mineral types available in Sri Lanka.

The physical and chemical properties of each clay and mineral type were investigated through literature.

The identification of suitable mineral nano material was done by using Computational Chemistry to collaborate with identified main clay type to make clay pottery. Gaussian Computer software was used to model clay and mineral type structures and to calculate the binding energies of each considering them as monomers. Then the binding energies were calculated by combining the modeled clay type with each mineral type by considering them as dimers. The clay and mineral combination with the most stable system shows the highest negative valued binding energy, was selected as the best collaborative material couple to use in cooking clay potteries.

In this study mainly analyzed for the nonstick property of identified clay and mineral combination by combining with fat /oil based on the binding energy by using Gaussian Software. The main types of fats which are saturated and unsaturated fat types and examples for each fat type were tested for the nonstick property by combining them with identified clay and mineral combinations.

1.5 Main Findings

The principal findings derived from the research are delineated as follows.

1. Red clay has been identified as the primary clay type utilized in the manufacture of cooking clay pottery.
2. Montmorillonite, Kaolinite, Graphite , Silica Sand, Quartz, Feldspar, Apatite, Mica, Ilmenite, Rutile, Zircon, Garnet Sand, Calcite and Dolomite has been identified as abundant clay mineral and mineral types in Sri Lanka.
3. The important chemical and physical properties of each clay and mineral type are described under the results and discussion through the collected via literature.
4. The Apatite mineral is the best mineral type to collaborate with Red clay due to it shows the most stable system with the highest negative valued binding energy -3177 Kcal/mol when combine with Red clay compared to other mineral combinations. Therefore, the best clay and mineral combination for the pottery mixture is red clay and apatite composite.
5. The binding energies when combine Red clay with saturated fat, unsaturated fat, coconut oil and vegetable oils are -1552, -2142, -2117 and -1522 kcal/mol respectively. These negative values indicate exothermic interactions, suggesting that the lipids adhere effectively to the red clay surface. In contrast, the binding energies, when combine Red clay and Apatite mixture with saturated fat, unsaturated fat, coconut oil and vegetable oils are 3212,

2376,2450 and 3903 kcal/mol respectively. Positive binding energy values denote endothermic interactions, implying that the combination of Red clay with Apatite reduces the sticking of fat to the clay mineral mixture. Thus, mixing Apatite mineral with Red clay enhances the nonstick property of clay and Apatite composite of the clay pottery.

1.6 Dissertation Structure

Chapter 1 outlines the introduction to the study, delineates the research gap, defines the research aims and objectives, summarizes the methodological approach, presents the key findings, and describes the overall structure of the thesis.

Chapter 2 delivers the literature relevant to the study. It provides literature regarding the hygienic problems of using metal and nonstick metal cookware, clay and minerals, advantages and disadvantages of using clay cooking pots, food stickiness, nano technology, computational chemistry and binding energy calculation.

Chapter 3 illustrates the methodology part for the data collection, combining clay and minerals, using Gaussian software under computational chemistry for modeling and binding energy calculation of clay and minerals and analysis part of the calculated data.

Chapter 4 shows the results and discussions obtained through the field visits, literature survey which was done for the clay and minerals, binding energy calculations and analysis part done for modeled clay, minerals and food fat/oil along with the research aim and objectives.

Chapter 5 consists of the conclusion, recommendations and Future works of the study for further extensive development based on these findings.

CHAPTER 2

LITERATURE REVIEW

2.1 Chapter Introduction

This chapter presents a comprehensive review of the existing literature to address the identified research gap and to establish a framework for the experimental procedures required to achieve the research aim and the objectives. Relevant literature was extracted regarding hygienic problems of using metal and non-stick metal cookware, food stickiness to the surface of the clay cooking pots, clay and minerals, computational chemistry and its usages, binding energy calculation and importance of applying nano technology in preparing clay and mineral composite for cooking potteries.

2.2 Hygienic Problems of Using Metal and Non-Stick Metal Cookware

The using of non-anodized or anodized metal cookware and non-stick metal cookware cause hygienic problems in human beings (Alabi and Adeoluwa, 2020; Geiger et al., 2014). The literature evidence of different kinds of hygienic problems and the causing activities for these health complications of metal and nonstick metal are demonstrated in this section.

2.2.1 Hygienic Problems of Using Metal Cookware

Currently many cooking utensils are made of different substances like aluminum, cast iron, copper, plastics, Teflon, stainless steel, clay, stones, glass and many metal materials (Shamloo et al., 2023). Various metal materials are used to manufacture cookware and utensils for cuisine purposes and aluminum, iron, stainless steel, silver, brass, gold and copper are some of metal constituents used for preparing those cuisine utensils (Alabi and Adeoluwa, 2020). Among those metal materials aluminum is considered as a cheap material and due to that reason aluminum cuisine equipment shows a high prevalence all over the world (Osborn, 2009). Using non-Anodized or non-coated aluminum pots causes many hygienic problems because of the discharging of aluminum metal ions and other material ions to the food when cooking. However, the usage of anodized or coated aluminum pots reduces the releasing of metal ions to the food when cooking due to the layer generated by the anodizing or coating process inside the pot. However, it is not a permanent solution, because with aging those anodized or coated layers are damaged by abrasing and scratching and cause food poisoning and then many health disorders. The discharging of metal ions to diet depends on the cooking time, temperature, PH level of the food and other material amounts when making the aluminum alloy cookware. There is a high possibility to migrate lead and arsenic into food from the aluminum alloy when damage to the coating (Alabi and Adeoluwa, 2020).

There are two types of heavy metals, biologically essential and non-essential. The heavy metals like Lead (Pb), Cadmium (Cd) Tin (Sn), Mercury (Hg) are biologically non-essential heavy metals and iron (Fe), Zinc (Zn) and Copper (Cu) are essential heavy metals. Essential heavy metals support relevant biological activities in the body and the amount should be at a sufficient level to maintain a non-toxic level due to excess amounts that may cause toxicity for the body. Non-essential heavy metals are not useful to any biological activities in the body and small amounts of these metals may cause toxic situations in the body (Slobodian et al., 2021). Therefore, the leaching of metal materials from the metal cookware directly affects the security and the quality of the food. Hence, the migration of heavy metals to the food from the cookware during cooking needs to be considered. The heavy metal migrating amounts can be measured by using the ICP device. The regular use of metal cuisine equipment leads to impairments and scratches of the vessel. Therefore, the release of heavy metal amounts inversely proportional to the usage time and the cooking time (Shamloo et al., 2023).

2.2.2 Hygienic Problems of Using Nonstick Metal Cookware

Non-stick cooking vessels are very popular kitchen utensils in the current society. The most specific thing is that a non-stick layer is coated in the inner surface of the pottery. Poly Tetra Fluoro Ethylene (PTFE) and Poly Fluoro Carbon (PFC) polymers are used as non-stick coating materials. The special characteristics of these polymers are the anti-sticking ability, mechanical properties like strength and the shallow ignitability (Ismaeili et al., 2022) and the major unfavorable characteristic is the weak abrasion resistance of these polymer coatings (Hatzikiriakos, 2012).

Metal vessels are used as substrate pots and the inner surface of these vessels are coated with Poly Tetra Fluoro Ethylene (PTFE) or Poly Fluoro Carbon polymer (PFC) polymers as layer to produce non-stick cookware (Coyle, 2023). Teflon is the commonly used name for Poly Tetra Fluoro Ethylene (PTFE) which is used to make non-stick cookware (Ismaeili et al., 2022).

Resistance to Rust, stickiness, heat, not reacting with food due to high mechanical strength of carbon and fluorine bonds and acting as a shielding, waterproofing, greasing layer are the major favorable characteristics considered to produce the non-stick vessels (Lee et al., 2007; Beckford et al., 2016).

Nonetheless the main disadvantage is, the PTFE layer starts to decline when the cooking pot heats up to 260 °C and completely decays over 350°C (Ismaeili et al., 2022). Also, ageing, cleaning for long time, rubbing and abrasions lead to remove or damage the non-stick layer as shown in Figure 2.1. Hence the lifetime of the nonstick cuisine utensil depends on the existence of PTFE non-adherent film. Another thing is that anti-sticking cookware is ideal only for very slight foods like meat slices, sausages, and egg. Though there is an anti-sticking layer in Teflon coating ware, food sticking occurs if used heavy food and it leads to damage to the nonstick film.

Therefore, it is not suitable for cooking heavy foods for long time in the same cookware (Coyle, 2023).

Figure 2.1: Damaging of nonstick layer of nonstick metal cookware (Shimizu et al., 2012)

With the heating during cooking, the PTFE layer starts to decay, and it emits minor toxic fumes. The increasing of the stove firing time during the cooking causes to increase the temperature of the nonstick cookware and then the overheating of the nonstick coating causes to break down the PTFE layer. With the overheating dangerous chemical gases are emitted as toxic fumes (Sajid & Ilyas, 2017) and breathing of these poisonous fumes causes the flu called "Teflon Flu" in the human body (Coyle, 2023) and for severe problems in the respiratory system (Lee et al., 1997) as in Figure 2.2. This "Teflon flu" also known as the "Polymer Fume Flu" and reveals many indications like fever, quivering, throat difficulties (Greenberg & Vearrier, 2015). Exposure to large amounts of polymer fumes cause severe damage in the lungs, body pains, heart pains (Shimizu et al., 2012).

Figure 2.2: Teflon fume and polymer/Teflon fume flu (Desk, 2024; Nurdin, 2024; Abdulla, 2024)

Perfluorooctanoic acid (PFOA) and Perfluoro Octane Sulfonate (PFOS) were used to produce PTFE (Teflon) until 2012 and, then the usage of PFOA and PFOS were prohibited due to their dangerous effect on the environment and human health

(Gerardu et al., 2023). PFAS is a poly and perfluoroalkyl substance which is used during the preparation of Teflon (Coyle, 2023).

Above mentioned PFOA and PFOS are the widely searched constituents of PFAS. According to probes and analysis it was identified that 98% of the community in the tested case with accumulated PFAS in their body in different levels in the United States. This poly and perfluoroalkyl substance including PFOA, PFOS and PFAS are completely artificial chemicals and the accumulation in human body for long periods of time creates bad health effects. PFAS is nondegradable and remains in the environment. These chemicals are deposited in organisms, and the concentration gradually increases during the lifetime. This is called "bioaccumulation". Then the bio accumulative chemicals are transferred to the top-level organism through food chains and food webs, and this incident causes "biomagnification" and severe health damages occur in life beings including humans (Geiger et al., 2014).

PFAS is used in many industries such as wetting agents, greases, food industry including the packaging industry, thin film manufacturing such as nonstick coatings for cookware (Geiger et al., 2014). During the manufacturing process PFAS, degradations, by products and contaminating substances are released to the water and soil. Releasing these chemical components leads to imbalance in the ecosystem and pollutes the environment. Water and soil pollution occurs, and consumption of polluted water leads to severe health problems in human beings like cancer and many diseases (Schaider et al., 2017).

Then GenX was invented as an alternative for the PFOA to use during generating Teflon (Gerardu et al., 2023) and it is generated by using "Ammonium salts" and Hexafluoropropylene oxide (HFPO) which is called dimer acid. This is a kind of Fluoropolymer and produced excluding PFOA and the major application of GenX is, it is used in a nonstick films manufacturing industry for metal cookware. According to the investigations done by the United States Environmental Protection Agency (EPA), GenX easily combines with water, and it has been detected in soil surface, air, and consumable water for drinking. However, PFOA has been replaced by the GenX and PFOS has been replaced by Perfluorobutane Sulfonic acid (PFBS) (US Environmental Protection Agency, 2018). PFBS is a substance of the PFAS family, and it is used to make nonstick layers for cookware as GenX (Wieck, 2023). PFBS also has been included in different water types such as effluent and drinking water and flooring detergents, polish, and wrapping industry. According to the studies conducted by EPA, it has been found there are bad health effects from GenX and PFBS. GenX causes bad conditions of human and animal liver, immunization system, kidneys, blood and express the symptoms of cancer conditions. PFBS consumption generates severe health conditions in thyroid, kidney, reproduction system and many organs in the body (US Environmental Protection Agency, 2018).

When considering present nonstick cookware, it is easy to clean, handle and food can be cooked without adhesion to the inner surface of the cooking vessel. The nonstick property is generated by applying a chemical coating on the inner surface and mostly using chemicals are PTFE and PFOA. The commercial name of PTFE is Teflon and the PFOA has been used to synthesis the Teflon. Both chemicals affect badly human, animal health and the environment. These nonstick chemicals reach up to higher temperature like 371 °C (700°F) within a short time of 3 or 5 minutes. With the increasing of the heat, 15 numbers of toxic and cancer-causing gases are emitted during the cooking. The inhalation and the deposition of these unfavorable gases lead to cancers, issues in infertility, testicles, liver, and pancreas in the human body. The International Agency for Research on Cancer (IARC) has been identified these nonstick chemicals PTFE and PFOA as "possibly carcinogenic to humans." (Bansal et al., 2020).

2.3 Food stickiness to the clay pottery

Food stickiness to the inner surface of the clay cooking pottery is an identified problem that leads to the development of proper nano material to use in cuisine clay pottery. The absorption of moisture and fat, fat composition of food, fat polymerization, fat melting, low-fat cooking and insufficient lubrication, porous surface, temperature control issues, insufficient seasoning and burning & residue formation (Adhikari & Adhikari, 2023, O'Neill et al., 2019, Hashemi et al., 2017).

Figure 2.3: Sticking foods in inner surface of clay pottery

Fats and oils exhibit stick property onto the surface of clay pottery due to the material's inherent porosity and the hydrophobic nature of these substances. The porous microstructure of unglazed or improperly sealed clay surface facilitates the infiltration and entrapment of lipid molecules within the interstitial spaces of the clay. This interaction is enhanced by the immiscibility of lipids with water, promoting their retention in the hydrophilic yet porous substrate. Clay materials can entrap lipid compounds within their particulate microstructure (Coxworth, 2018). Therefore, the sticking characteristics of a material are influenced by its physical state, whether amorphous or crystalline, which is governed by its chemical structure as well as the molecular organization and motion within its structure (Dopfer et al., 2013).

In food processing, food sticking to the preparing vessel surface is a familiar issue, especially during preparing bakery, rice and other dehydrated foodstuffs. It leads to loss of food content due to sticking and reduce the durability of the vessel because of frequent cleaning and accelerating ware. Sticking causes overheating, sensory defects, and reduces food quality. Bacterial activities occur on the sticked food due to improper cleaning of surfaces, and it causes food contamination (Caroline et al., 2021). Further the fatty food sticking to the surface carries significant economic implications. Residual deposits increase the recycling costs due to the enhancement of waste vessels and refining expenses, particularly for high-fat meals. In addition to that, the reduced food quality with poor appearance can be arisen due to food stickiness (Michalski et al., 1998).

Seasoning is the current available process to improve the quality of the cookware including the nonstick property to implement initially before it uses to cook at first time and it is a disturbance to the busy life. Seasoning of clay cooking pot enhances its structural integrity, strength and functional performance. This procedure conditions the porous spaces of new clay vessels, reducing the risk of breaking and developing thermal retention. By filling micro-pores, seasoning builds a non-stick layer, decreases food adhesion, and promotes uniform heat supply. Overall, it increases cookware's durability and cooking efficiency (Adminecoveya, 2025).

Therefore, modifications are required to avoid the stickiness between the pottery surface and the food (Saikhwan et al., 2006).

2.4 Clay and Clay Minerals

Clay is generated in a natural way, and it consists of fine grain size small particles, characterized by its plastic behavior at certain moisture levels and its ability to undergo hardening upon drying or thermal treatment. Clay generally consists of "phyllosilicates" and in addition to that, clay is included with accessory mineral phases that cause the absence or presence of plasticity, organic materials and for other characterizations. According to the ISO Standard 4688:1996 the grain particle size less than 0.004 mm is considered as clay (Al-Ani& Sarapaa, 2008).

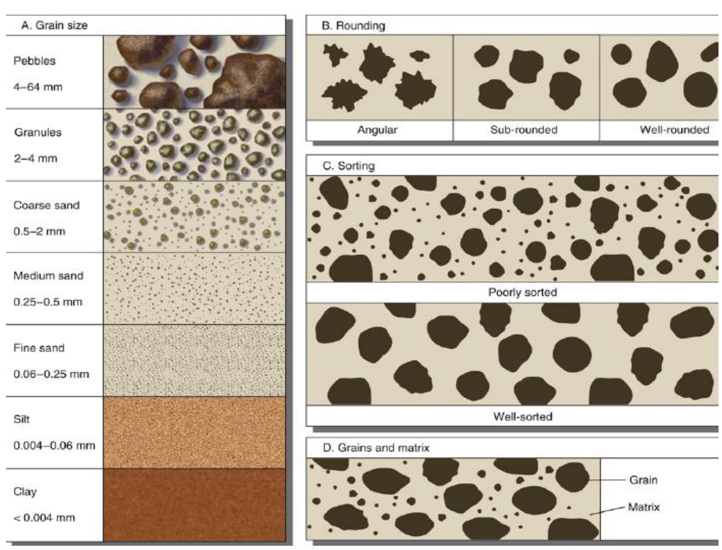


Figure 2.4: Classification of soil grain (Al-Ani& Sarapaa, 2008).

Moreover, clay basically originates from raw minerals, having different types of geometry and morphology. It has hexagonal crystal structures, and they are deposited as horizontally leveled hexagonal sheets by connecting each plate by water. The layered structure of clay minerals allows the individual sheets to slide past one another when hydrated, resulting in the material's characteristic plasticity under wet conditions (Bloomfield, 2016).

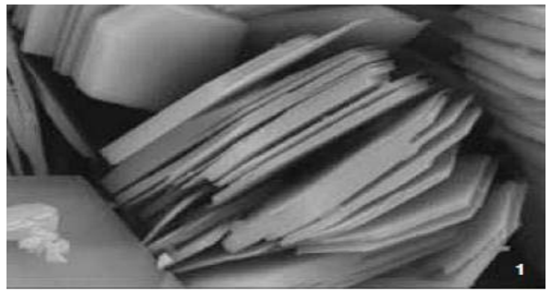


Figure 2.5: Hexagonal crystal structures (Bloomfield, 2016)

Clay minerals are defined as phyllosilicate minerals, as well as other mineral species that generate plasticity to clays and exhibit hardening behavior upon drying or thermal treatment. Clay minerals are called “sheet silicate” and they belong to the class of layered phyllosilicates typically formed as secondary products through the chemical weathering and hydrothermal alteration of primary silicate minerals at the soil and commonly known as sedimentary rocks. Further clay minerals function as chemical sorbents, capable of retaining water and adsorbing dissolved plant nutrients released through the weathering of primary minerals. Major clay and clay minerals accumulations modes are primary clay depositions and Secondary clay depositions (Al-Ani& Sarapaa, 2008).

Primary clay depositions- Deposition of the clay remainders at the same location that it was created called primary deposition.

Secondary clay depositions - occur by transporting clay from the originated location to another site through water flow and accumulate them as a new sediment. Wetlands and lakes are considered as secondary sedimented clay rich sites.

Clay minerals differ greatly from one another, even though they all are built up with octahedral and tetrahedral sheets as their fundamental construction units. The changes in organization and composition of these sheets are responsible for the variations in their physical and chemical properties. The development and the identifying of crystal structures of these clay minerals are mainly based on the ions O^{-2}(1.40Å), OH^{-1} (1.41Å), Al^{+3} (0.55Å), and Si^{+4} (0.41Å) due to clay minerals are hydrous aluminosilicates (Al-Ani & Sarapaa, 2008).

2.4.1 Types of Clay and Clay Mineral types in Sri Lanka

Sri Lanka is rich in diverse types of clay, which are derived based on their use in making different types of clayware. The three main types found across Sri Lanka are earthenware clay, ball clay, and white clay. Earthenware clay, typically called red clay, is mixed with sand and grit to make bricks and is sourced mainly from the Naththandiya area. Its purified and seasoned layers are used in the pottery industry. Ball clay, available in large quantities in Boralesgamuwa and Meetiyagoda, is primarily used in the production of ceramics and porcelain (Export Development Board Sri Lanka, 2021).

Mainly identified clay minerals are kaolinite, Montmorillonite, Vermiculite, Illite, Chlorite and Palygorskite in the world (Al-Ani& Sarapaa, 2008). Nonetheless Kaolinite, Montmorillonite and Micaceous are the major clay mineral types existing in Sri Lanka. When considering industrial minerals Graphite, Ilmenite, Rutile, Zircon, Quartz, Feldspar, Kaolin, Apatite, Silica Sand, Garnet sand, Mica, Calcite and Dolomite are the identified non-metallic minerals in Sri Lanka (Export Development Board Sri Lanka, 2021).

Figure 2.6: Industrial mineral material in Sri Lanka (Export Development Board Sri Lanka, 2021).

2.4.2 Clay Pottery Industry in Sri Lanka

The Sri Lankan clay pottery industry has an archeological value, and many excavations were done in Dry Zone, Anuradhapura and Jaffna have been revealed the consumption of these pottery since the early stage of this island’s history. This industry contributes to the national economy by providing around 30% to the Gross Domestic Product (GDP) and provides employment for about 25% of the total employees. Mainly this is formed as village industry and currently the clayware centers are established at Ampara, Anuradhapura, Badulla, Batticaloa, Gampaha, Hambanthota, Jaffna, Kaluthara, Kandy, Kegalle, Kilinochchi, Kurunegala, Mannar, Matara, Monaragala, Mullativu, Puttalam, Rathnapura and Vavuniya Districts (Asia InCH, 2017).Table 2.1

shows the product range of clayware in Sri Lanka categorized under four main categories.

Table 2.1: The product range of clayware in Sri Lanka (Asia InCH, 2017).

Category	**Product**
Household and Ritualistic	Cooking clay potteries, Guruleththu, Haliya
Tiles and Architectural items	Clay tiles in different designs
Decorative items	Terracotta pots, Clay pots, food containers
Motifs and designs	Decorative items – animal, flower, geometrical designs

Earthenware clay (Red clay), Ball clay and white clay are the abundant clay types in Sri Lanka, and they are used in making pottery, ceramic and other clayware (Export Development Board Sri Lanka, 2021).

Figure 2.7: Types of clayware in Sri Lanka (Nandadeva, 2017)

2.4.3 Using Clay in Pottery Making

World history has discovered the usage of clay pottery for cooking purposes in many countries all over the world under different traditions. The availability of the favorable characteristics in clay for use human consumption leads to using them in making clay potteries. They are (Trivedi et al., 2017; Amboro et al., 2023; Newbasics, 2021),

- Clay's ability to even heat and moisture circulation during cuisine enhance food preparation and food tasty with fresher and more tender. Further the curve underneath the clay vessel improves the area exposed to heat and develops efficient heat circulation along the surface.
- It consists of essential natural nutrients and vitamins beneficial to human health such as Calcium, Phosphorous, iron, magnesium and sulfur.

- Clay has its natural alkaline property which leads to balance the acidity in the food, and it causes better food digestion.
- Natural cooling ability as a sustainable cooling method without using electricity of the clay pot.
- Clay pots are completely environmentally friendly, harmless and act as a natural detox.
- Proficiency at filtering water and eliminating contaminations.
- Ability to eliminate turbidity and reduce water discoloration.
- Clay is inflammable, resistant to heat and corrosion.
- The plasticity ability under proper heat supply and moisture of clay facilitate making clay pots and other types of clayware with different shapes.

Contrast to above advantages there are some disadvantages of using clay for pottery. They are listed as follows. (Newbasics, 2021; Amboro et al., 2023)

- Mold and Fungus growth on pot surfaces due to sticked food parts, insufficient drying conditions and cleaning issues.
- Fragile property leads to difficulties in handling clayware.
- Seasoning needs to be done before initial use to protect the durability and to enhance the nonstick property of clay.
- Low tolerance to the speedy temperature fluctuations and it directs to fracture the clayware.
- Difficulty in washing and cleaning of clay potteries due to porosity. The cleansing chemicals penetrate porous spaces and the discharging of these chemicals into food in subsequent cooking.
- Slow cooking time

2.5 Nanotechnology

The word “nano” in the term nanotechnology, implies one part of a billionth ($1x\ 10^{-9}$) (Poole & Owens, 2003). There is a special terminology combining with the word “nano” according to the British Standards Institute (BSI 2005), the United Kingdom Royal Society and the Royal Academy of Engineering. Nanoscale, Nanoscience, nanotechnology, nanomaterial, nanoparticle, nanocomposite, and nanostructure are the most essential vocabulary which is used in nano related experiments and activities (Public Health, 2006).

2.5.1 Applications of Clay Nano Particles

There are naturally available and artificially generated nano clays with nanoparticle dimensions from 10-100 nm. The nano clay is consisted with silicate layers built up of these nanoparticles (Kausar, 2020). Nano clay is used to create compositions with collaboration with other materials, and it gives composites with improved properties which are its structural permanency, ability to swell, expanded interlayer distance, high hydration potential, and strong chemical motion (Sharma & Joshi, 2023). Mainly montmorillonite, bentonite, kaolinite, hectorite, and halloysite are considered as naturally available nano clay types depend on their chemical arrangement and structural forms (Dhiman et al., 2022).

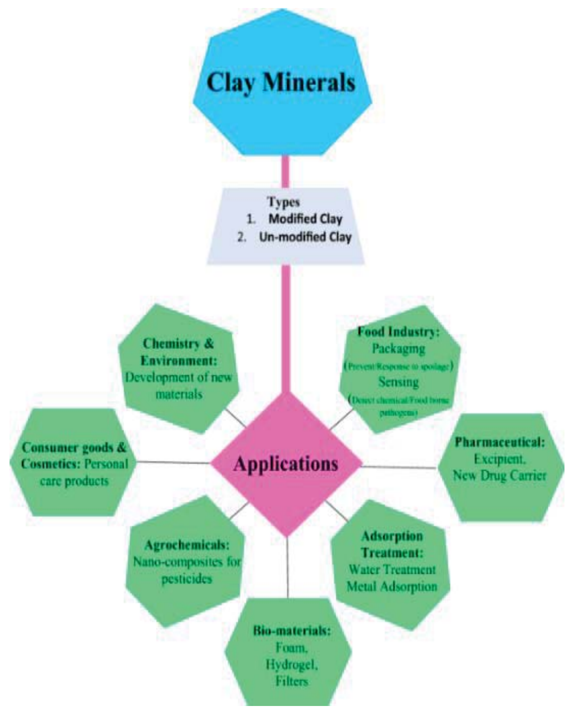


Figure 2.8: Applications of Nano Clay (Awasthi et al., 2019)

Nano clay materials consist of exceptional performances in the characteristics and properties than their native raw states. They are superior surface qualities, increase catalytic performance, improved barrier and abrasion properties, higher tensile strength, low thermal expansion, very good processing properties, act as nano-adsorbent to absorb harmful materials (heavy metals, dyes, antibiotics), high removal efficiency and loading of harmful chemicals in water, remedy the corrupted water and act as a property enhancer of effectiveness and efficiency for water refinement (Awasthi et al., 2019; Nanografi Advanced Materials, 2019 ; Isaifan et al., 2013).

Currently Nano clay has many applications in various industries due to their extraordinary physical and chemical properties. They are in, (Awasthi et al., 2019; Bantie et al., 2024; Ntim et al., 2018)

- Nonstick cooking surfaces- Nanoparticles which are made from silica, Titanium Dioxide and nano clay are used as a nanocomposite in making cooking utensils such as ceramic, oven, frying pans. According to the scenario the utensils are prepared by using completely with nano composite or by applying as a nonstick coating on the surface. Although this application enhances the nonstick property the investigations are implemented to investigate the nanoparticle leaching into the food.
- Adsorption treatment sector- It is used as a nano adsorbent in the water treatment and metal adsorption sector due to its excellent ability to absorb impurities, heavy metal and toxic materials. Therefore, nano clay is used for water purification and filtration units.
- Food Industry - It is used for Food packaging and to value add to plastic packaging planes as a filler material. Incorporating nano clay into plastics enhances tensile strength, boosts blockage and abrasion resistance, improves surface finish, reduces thermal expansion, and provides excellent flow and preparation characteristics.
- Chemistry and environment - Not only that, nano clay is also involved in energy, industrial operations, manufacturing sensors and various ecological applications in many industries.
- Geopolymer and construction Industry- Moreover, nano clay is used to create geopolymers and in the building and construction industry, using nano clay as a mixing material in relevant ratios and concentrations with concrete enhances its chemicals and physical characteristics. It is one of the suitable time saving methods for producing building stuff economically and it leads to improve durability, productivity, and overall operation in raw material manufacturing. The nano clay integration with concrete significantly enhances the strong mechanical and chemical properties, decreases shrinkage, inflammability, thermal and gas barrier properties and mitigates the draining and separation.

  In road development activities, nano clay is used to property improvement of asphaltic compounds, and it causes surface improvement of roads.
- The pharmaceutical sector- Kaolinite type is used in the medical sector for pharmaceutical drug formulation, for gut-active adsorption and for many medical treatments.
- Agrochemicals sector- nonmetallic minerals which belong to the mica family are utilized as an agrochemical to improve ground level potassium level to improve the fertilizer supply to crops. Montmorillonite and kaolinite are applied in the process of pesticide preparation.

Moreover less, biomaterials and consumer goods and cosmetics are some other industries that use nano clay.

2.5.2 Synthesis of Nano clay and composite

There are two main methods to synthesis nanoparticles (Abid et al.,2022).

1. Top-Down method
2. Bottom-Up method

The top-down method involves declining larger materials to nanoscale dimensions by using mechanical operations, whereas the bottom-up method builds greater nanostructures by chemical transformation method assembling them from individual atoms and molecules. The figure below shows the techniques which are used under each method.

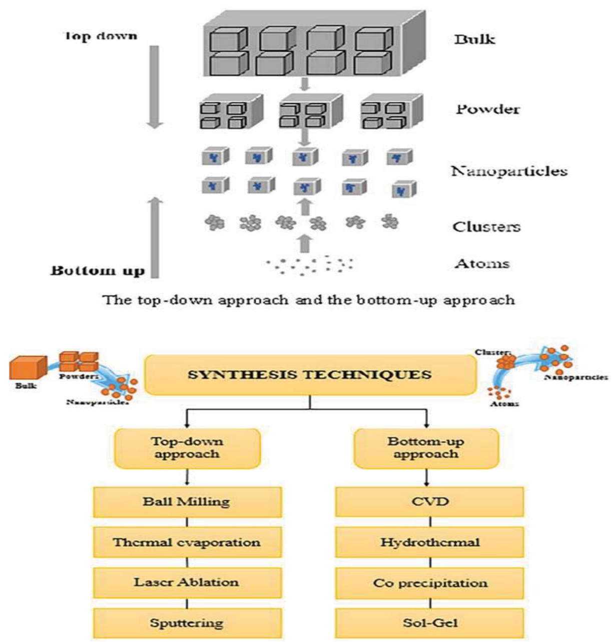


Figure 2.9: Nano particle synthesis methods (Abid et al.,2022)

Ball milling and ultrasonication are the main Top-down techniques which are applied for making nano clay. According to that there are no specific synthesis processes and mechanical operations, and high frequency sound waves are applied to exfoliate individual silicate layers of clay accordingly. Simultaneously hydrothermal synthesis, precipitation and Sol-Gel techniques are used to prepare nano clay by involving chemical synthesis. (Abid et al.,2022).

Nano clay is applied as composite based applications at industrial level and the main composites are polymer base, metallic base and ceramic based nanocomposites. Under these main methods there are various types of techniques to synthesize nano clay composites (Awasthi et al., 2019; Nanografi Advanced Materials, 2024).

- Solution Blending
- Molten State
- Polymerization
- Liquid nano clay

2.6 Binding Energy (BE)

Binding energy is calculated to find out the adhesion properties of aggregate mineral substrates by using system energy and the energies of each single molecule. Binding Energy is considered as the negative (-) value of the intermolecular interaction energy. A greater BE indicates more powerful interaction between the molecules, resulting in a steadier system (Du & Zhu, 2019).

When generating a nucleus by combining two separate nucleons which are proton and neutron, the system energy is decreased, and the change of that energy is always getting negative (-) value due to the generating of a more stable system than individual sub atoms. That changed energy value is called Binding Energy, and it can be defined as, "Released energy when combining a molecule or atoms with another molecules or surfaces" (Zhang et al., 2023).

In another way the Binding Energy can be described as, the entire energy of the nucleus/molecules consisting of the certain subatomic particles which are proton and neutron is lower than the collective entire energy of the detached subatomic parts for the same and this energy change is called the BE of the system. In other words, Binding Energy is equivalent to the necessary energy amount for binding the nucleus with protons and neutrons or separating the nucleus into detached protons and neutrons (L'Annunziata, 2016).

The formula below is used to calculate Binding Energy (Du & Zhu, 2019).

$$\mathbf{E_{bind} = -E_{inter} = -(E_{ab} - (E_a + E_b))}$$

Binding Energy -E_{bind}

Total energy of the combined system – E_{ab}

Intermolecular interaction energy of the system – E_{inter}

Energy of a monomer – E_a

Energy of b monomer - E_b

According to the above equation, binding energy is determined by calculating the difference between total energy of the AB compound and the accumulation of the total energy of monomers A and B (Du & Zhu, 2019). The intermolecular interaction energy is also characterized by Binding Energy (Zhang et al., 2023).

These nucleus/ molecules formations and breakdowns perform as exothermic reactions and endothermic reactions. An Exothermic reaction has occurred with negatively changed energy ($-\Delta H$) by forming a more stable system/product by releasing energy to its surroundings. If the changed Energy positive ($+\Delta H$), an Endothermic reaction has occurred by absorbing heat from its surroundings while forming a less stable system/product (Karthik et al., 2024).

2.6.1 Factors affecting Binding Energy

There are various factors which affect the binding energy of a system, and they are particle size, structural arrangements, the oxidation state of the material, chemical properties, physical properties, geometrical factors, system electronic charge density, trepidations, and type of interactions between the substrates (Radnik et al., 2002).

When considering the particle size of the material, it has a substantial effect on the binding energy and there is an inversely proportional relationship between particle size and binding energy. When the particle size is small, the system binding energy is increased. Therefore, using nanoparticles leads to generating high binding energy of the system with strong intermolecular interactions and a steadier system (Wang & Zhao, 2013).

Literature shows that the molecular simulation options coming under computational chemistry are implemented to predict the information regarding physical and chemical properties before starting the physical experiments of Montmorillonite and different types of clay and materials. According to that the material structures, binding energies, interaction energies and other relevant possible properties are predicted by using specific software (Toth et al., 2004).

2.7 Computational Chemistry

Computational chemistry comprises intense realistic elements. The fundamental function of this field is converting the relevant theoretical applications into performing computer programs by using a particular computer software with respect to generate the end results. The major focusing areas of this application are forecasting and calculating the chemical structure and energy of the relevant molecules. Relevant resources in computational chemistry and modeling software are used to achieve the above activities and simulation (molecular dynamics) is a progressively impressive function in the computational chemistry field. Compatible applicability is a considerable factor of the specific computational resources and modeling software when use for calculations due to it shows specific performances in order to the specific applied algorithm (Jensen, 2017).

However Computational chemistry is a rapidly evolving field which is used for modelling and simulating the chemical systems of molecules. Therefore, this is a very important discipline which can be applied to resolve different types of chemical and biochemical matters and to explain and predict physical and chemical properties of modeled and simulated molecules. The foremost calculations done by using computational chemistry are bonding energies of molecules, energy of the modeled molecules, changes of energy and the structures at conversion condition, energy and the pathways of molecular reactions, molecular and atomic movements, generating spectra such as NMR, CD and IR and RAMAN spectra. At the same time computational chemistry is used for determining properties such as thermodynamics, modeled plains', magnetic and including many chemical and physical properties of molecules (Ramachandran et al., 2008).

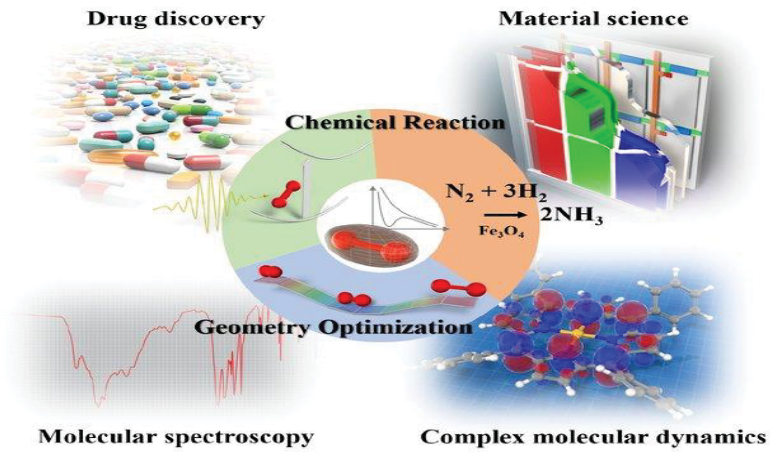


Figure 2.10: Application of computational chemistry (Shikano et al., 2020)

Meanwhile High time consumption is a main issue when synthesis of chemicals and polymers in the laboratory facilities, specially "Molecularly Imprinted Polymers" and because of that, substantial absorbing of diluents and chemicals are occurred. Therefore, the accuracy of the result of the reaction is affected by those factors. Hence computational chemistry has become an important field for resolving various matters in the chemical field through simulation and modeling (Marć et al., 2017).

2.7.1 Theories Apply in Computational Chemistry

Computational chemistry software is generated involving five types of methods and theories which are Density Functional Theory (DFT), Molecular Dynamics (MD), Semiempirical methods, Molecular Mechanics, and Ab initio calculations (Admin, 2024). Among these methods and theories DFT is playing a key role in computational quantum chemistry discipline. DFT type can be introduced as a method of quantum mechanical, and it is used for analyzing and evaluating the electronic structure including electron distribution of atoms, molecules, and solid objects. Physics and chemistry are the main subject areas that use the DFT. Diffusion is a major issue when reactions occur in a larger system. However high energy can be accumulated during significant atomic and molecule aggregations. Therefore, the application of DFT is influential for systems like nanomaterials, supramolecules chemistry, biochemistry etc. (Mourik et al., 2014).

Molecular dynamic (MD) theory is another important type which is applied in computational chemistry software. MD means simulation and its main functions are to calculate and forecast the movements of the atoms in the molecular system (Hollingsworth & Dror, 2018), estimate and analyze the binding and kinetic energy of interfaces and select the most proper molecules for generating more stable molecules for the enhancement of the system (Salo-Ahen et al., 2021). When considering the industry applications of MD Simulation, it is an important discipline in minerology (Greathouse & Cygan, 2013), drug and pharmaceutical industry (Salo-Ahen et al., 2021), health sector, food and agriculture and many valuable disciplines (Nian et al., 2021). At the same time MD simulation plays a significant role in improving and formulating nano and crystalline materials (Salo-Ahen et al., 2021) according to theoretical and technological improvements. As well as MD simulation is a valuable application to predict the crystal structural arrangements, atomic behaviors, and the dynamic temperaments of clay minerals. Most importantly molecular simulation process is a regularly advancing method to use most appropriately in providing distinctive understanding about interlayer and surface procedure mechanisms of clay minerals, to create simulative conceptual models and assumptions to predict chemical and the physical properties and to use as a novel software tool in modeling and analyzing the nanomaterial properties in minerals than the existing typical techniques (Greathouse & Cygan, 2013).

Ab initio calculations are used to find out the major elementary properties according to the quantum mechanics theories. It gives precise outputs for the entire energy for the solid system including or not faults and calculates the uppermost concentration of the contaminations during the thermodynamic equilibrium. This precisely computes the interatomic and undersurface relations and forces, electronic density while considering the chemical and magnetic impacts in the system and this leads to generate most exact modeling and create a substantial ability to predict the substance properties. Further the Ab initio method is appropriate as above DFT and MD theory to apply for find out the properties of nano scale systems (Odegard, 2017).

Semiempirical method is originated from "Hartree-Fock or Density Functional Theory" by doing methodical calculations and it is heading to generate a more effective calculation method which is quicker than the ab initio method (Christensen et al., 2016). Though this is seen as a similar theory as ab initio method semiempirical method is differentiated by more focusing on dropping the calculation time by avoiding the time utilizing two electrons' integrals and these assumed calculated values are used as the analyzed data for the final calculations. Also, this decreases the more complex calculations in the system to a significant range (Ramachandran et al., 2008). Therefore, the semi-empirical method fulfills its computational part with the feeding of experimental data to parameterize all materials of the molecular structure (Johansson et al., 2012).

Molecular Mechanics (MM) theory is used to compute the entire energy that is contained in the whole molecular system, and it is considered as a calculation of bonding energy, electro statistic and binding energy including van der Waals bonds. This computational method generates higher accurate straight calculations similar to ab initio theory which is needed for molecular modelling. This is an empirical method that computes the qualities and properties like geometry, strain, standard enthalpy of forming, frequency of vibrations, polarity of the molecule system (Abdelrasoul et al., 2017). Mainly this defines the energy of "bonded atoms" in the molecular system which are van der walls interactions and electro statistic energy in force between negatively or positively charged atoms called coulombic interaction. The accuracy of the molecular modeling done by using molecular mechanic theory depends on the significant level of changeability of geometrical parameters of relevant molecules that affect interactions (Hehre, 2003). However, this theory involves different types of computational chemistry modeling software due to decreases the complications in calculations in modeling and it accepts the molecular simulation process of substantial chemical systems for prolonged periods.

2.7.2 Application of Computational Chemistry Tools in Modeling

The quantum chemical calculations in computational chemistry are done by involving proper software and tools. Molecules modeling and simulation activities are completed by using this quantum chemistry software which consists of the applications of the theories, density functional theory (DFT), molecular dynamics (MD), semi empirical methods, molecular mechanics, and ab initio calculations. Therefore, the most accurate approximate quantum chemistry calculations are graphically represented by proper computational software (Lehtola & Karttunen, 2022).

A methodically arranged computer system is used to answer the theoretical formulars in computational chemistry according to the relevant molecular activity, to describe the chemical incidents and to interpret and predict the physical and the chemical properties of the relevant molecular system. This field plays a significant role as an independent method which can be associated with other multidisciplinary scientific research in different fields. There are various kinds of computational programming packages available in the field and major categories of the licensing are for open sources software tools, academic purpose software tools, commercial purposes and governmental programming tools. (Adhikari & Adhikari, 2023). There are different types of computational chemistry software which are Gaussian, GAMESS, Dalton, DIRCCR12, Psi3, Jauguar, SAPT, Molpro, Spartan and Quantum Expresso (Malyshkina & Novikov, 2021).

2.7.3 Using Gaussian Software in Research Work

Gaussian is a computational chemistry software used by chemists, chemical engineers, biochemists, physicists, and other researchers to explore both traditional and cutting-edge areas of chemical research (Pittsburgh Supercomputing Center, 2024). The GS is used in quick assessments of molecular similarity to compare the molecular electrostatic potentillas (Good et al., 1992). Moreover, Gaussian is a widely used computational chemistry tool in materials science, helping researchers simulate material properties, analyze chemical reactions, and explore structural characteristics (Lee, 2025). Furthermore, research has been conducted for analyze the adsorption of coal and methane at the molecular level using Gaussian simulations. Gaussian was employed to build and optimize molecular models of four coal types which are lignite, sub-bituminous, bituminous, and anthracite. The simulations provided data on their interactions with methane, including optimized adsorption structures, binding energy, bond lengths, vibration frequencies, and infrared spectra (Yang et al., 2024). When considering another way of using GS in analyzing adsorption property, the Gaussian simulation method is one of the rapidly evolving theoretical approaches. It provides details such as molecular structure, charge distribution, and atomic binding energy and studies were carried out to simulate and analyze the CO_2 adsorption performance of the absorbent by using GS due to its reliable predictive capabilities (Tang et al., 2011). On the other hand, Gaussian is used in food industry sector to analyze a triglyceride molecule composed of palmitic, oleic, and stearic acids, derived from waste animal fat, which participates in the transesterification reaction involved in biodiesel production (Srinivasan et al., 2020).

The characterization and mapping of mineral compositions by using Gaussian models is another application of GS in industrial residues is gaining attention, as it can offer valuable insights into processing activities at such sites and their environmental impact (Marion & Carrère, 2018). GS is a quantum method which can be used in mathematical modeling of crystal properties and structures (Matyszczak et al., 2025).

This software enhances the efficiency of molecular electronic structure calculations. Gaussian enables the prediction of various molecular properties, including Raman and IR spectra, molecular energies, vibrational frequencies, atomic charges, transition state geometries, NMR shielding constants, and magnetic susceptibilities. It incorporates a wide range of scientific and modeling capabilities, and its calculations are only restricted by the available computational power and time, with no artificial constraints imposed by the software itself (Malyshkina & Novikov, 2021).

Moreover, the Gaussian basis method plays a leading role in the quantum chemistry field. The special characteristics of Gaussian tool are the entire electrons in the molecular system are included in the calculations and these calculations and the analytical evaluations of electrostatic properties between electrons and electrons densities (Columb Integrals) are done effectively and accurately (Lehtola & Karttunen, 2022).

The benefits of using Gaussian Network Model (GNM) are, it is not only applicable to tiny molecular structures and particular solo molecules as well as to large, complex and combined molecules. The advanced controlling capability with optimization and frequency calculation directs to the accurate and speed simulation of the relevant molecules (Gaussian.com, 2019). Then it provides the results within a short period of time. The calculation process is done within a very low duration compared to other existing computational modeling tools (Yang et al., 2006). Further, Gaussian can be applied in all three primary phases gas, liquid, and solid (Ritme, 2025) and serves as an effective tool for analyzing the crystalline structures of minerals (Marion & Carrère, 2018).

Mainly the Gaussian Software consists of three main interfaces which are Job Processing window, Gauss view interface, graphical interface (Gaussian.com, 2019).

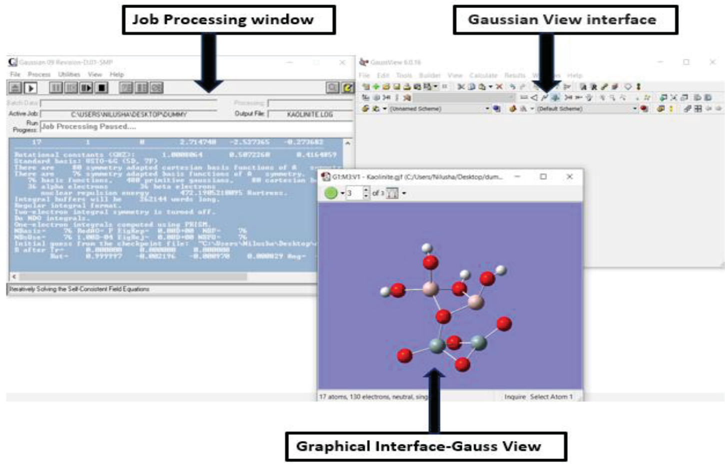


Figure 2.11: Three main interfaces of GS (Gaussian.com, 2019)

2.8 Relationship Between Edible Fat / Oil and Food Stickiness

As mentioned previously fat and oil content in foods are cause to stickiness of food to the cooking pottery surface and they have versatile usage in food industry. Therefore, widely using food type, fat and oil in food industry is providing considerable contribution for the food stickiness during the food preparation.

According to global food consumption and food fortification process oil and fat are important in cooking due to enhancement of nutrient absorption, flavor and texture, heat transfer and even cooking, act as a cooking medium and versatile usage in food industry (Mannar & Wesley, 2025).

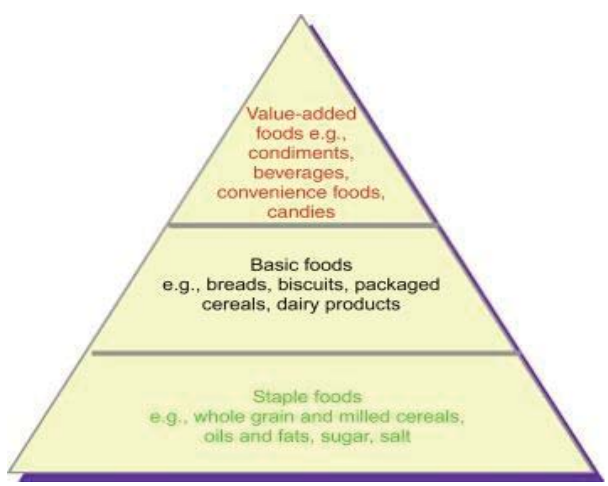


Figure 2.12: Fortification food product pyramid-Standard food vehicle for staple food (Mannar & Wesley, 2025)

There are two types of fat and oil which are saturated fat and unsaturated fats. Saturated fat has straight hydrocarbon chains without double bond between c-c atoms. Coconut oil, palm oil, Butter, ghee, cheese, full-fat dairy products, fatty cuts of meat and other relevant fat/oil types are included in the saturated category. Unsaturated fat is existing as monounsaturated with one double bond between carbon atoms and polyunsaturated fat is existing with more than one double bond between carbon atoms. These both types are in Cis and Trans forms. Vegetable oils (olive, canola, sunflower, soybean, etc.), nuts, seeds, avocados and Fish oil are rich with unsaturated fat/oil (Ginneken et al.,2019; Harvard T.H. Chan School of Public Health, 2014).

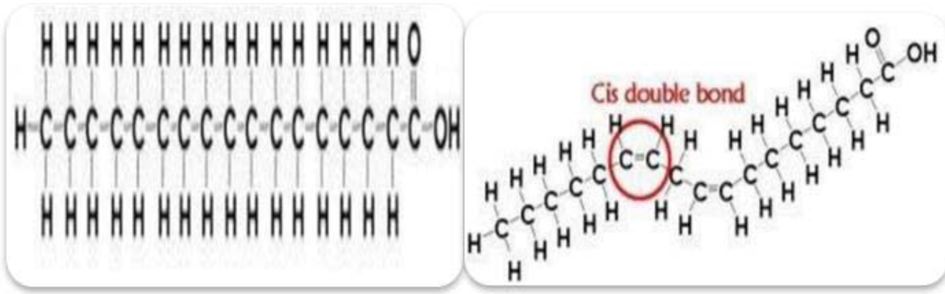


Figure 2.13: Saturated and unsaturated fat/oil (Ginneken et al.,2019)

Fat/oil are derivated from fatty acid and glycerol and they are described as triglycerides. These triglycerides can be performed as simple or mixed triglycerides according to the fatty acid types, whether saturated, monounsaturated or polyunsaturated (Patterson, 2009).

2.9 Summary

This chapter discusses the relevant literature aspects towards the developing of proper nano material to collaborate with clay in making cooking clay pottery which are hygienic problems of using metal and non-stick metal cookware, food stickiness to the clay pottery, clay and clay minerals, types of clay and clay mineral in Sri Lanka, clay pottery industry in Sri Lanka, using clay in pottery making, nanotechnology, applications of clay nano particles, synthesis of nano clay and composite, binding energy (BE), factors affecting to binding energy, computational chemistry, theories apply in computational chemistry, applications of computational chemistry tools in modeling, using gaussian software in research work and relationship between edible fat / oil and food stickiness.

This starts with the reasons illustration related to the research gap identification which are the occurrence of hygienic problems in the human body because of the usage of metal and nonstick metal cookware and the food stickiness during the cooking process to the inner surface of the clay pottery. Though there are advantages in using metal nonstick cookware, the health effect such as "Polymer fume flu", carcinogenic situations and other relevant health disorders have occurred by using anodized or non-anodized metal cooking vessels and the nonstick cooking vessels with the Teflon (PTFE), PFOA, PFOS, PFAS, PFC chemicals. However, even if clay pots are used instead of metal cooking vessels, due to the health and other benefits with clay, there should be property improvement as suitable for current busy lifestyle with improved nonstick and other relevant properties.

The nonstick clay pottery making material development process is discussed by using the most usable clay types and natural industrial nonmetallic minerals in Sri Lanka. Red clay, Ball clay, and White clay are the most usable clay types in clay industry in Sri Lanka. Kaolin, Montmorillonite, Graphite, Ilmenite, Rutile, Zircon, Quartz, Feldspar, Clay, Kaolin, Apatite, Silica Sand, Garnet sand, Mica, Calcite and Dolomite are the abundant industrial nonmetallic minerals in Sri Lanka. As Sri Lanka is a natural clay and mineral rich country the abundance availability of these materials is an advantage for maintain the cooking clay pottery industry as ancient and village industry. The Red clay is the most usable clay type in Sri Lanka for use in cooking pottery industry. The mineral material collaboration with Red clay is considered as a property improving strategy and using nano materials in suitable method of this pottery making clay and possible mineral material is a proper way to enhance the nonstick property of the materials.

The importance of using computational chemistry for identifying the proper mineral material to collaborate with clay is conversed. Using Gaussian software under computational chemistry is an appropriate method to identify the proper mineral material through the simulation process. Molecules modeling and the calculation BEs between clay and mineral material through the simulation in Gaussian software provide the predicted values and abilities to identify the best clay and mineral combination. Particularly the binding energy predicts the suitability of the collaborative mineral material to the clay for making the clay cooking pottery. This process is appropriate as it predicts valuable information prior to implementing the actual experiments in laboratory facilities. This is a time and a resource consumption reduction process than the actual experimental works.

Fat/oil plays a major role in the human diet. Therefore, fat/oil is used in investigating the nonstick property performances by involving the Gaussian software through finding BEs. These findings through the Gaussian calculations provide significant value in planning the implementation of an actual experimental process to make the nonstick clay pottery clay and mineral material.

CHAPTER 3

METHODOLOGY

3.1 General

This chapter describes the methods that were implemented for developing proper nanomaterial to use in cooking clay pottery making. According to that, the data collection methods and activities using interviews through questionnaires, literature review on research gap identification and properties identifying of clay and minerals, designing the models of relevant clay and mineral types using Gaussian software (GS), simulating modeled molecules and calculation of binding energies of relevant individual clay and mineral molecules (monomers) and clay mineral combination (dimers) to find out the best appropriate mineral to combine with clay to use in clay pottery and data analyzing regarding the performance of identified clay mineral combinations for the nonstick property are included in this chapter.

3.2 Research Methods

This research methodology is mainly aligned according to two aspects which are research gap identification and experimental methodology. The research gap identification was done in the introduction part based on the literature review part towards fulfilling the objective, Identify the industrial need of developing a proper nano material to use in clay pottery which is used.

The Experimental methodology consists of four main steps to achieve the objectives, Identify the proper material which can be used as a nanomaterial for clay pottery and analyze the performances of the identified clay and mineral combination for nano composite. They are Collecting Primary and Secondary Data, finding out the physical and chemical properties of each clay type and clay minerals, identify a suitable nano material to apply for clay potteries and analyze the performances of the identified clay + Mineral combination for nano composite.

The complete research methodology is shown in the below Figure 3.1 and the research methodology consisting of all activities which were completed during the study is shown in the research design below Figure 3.2.

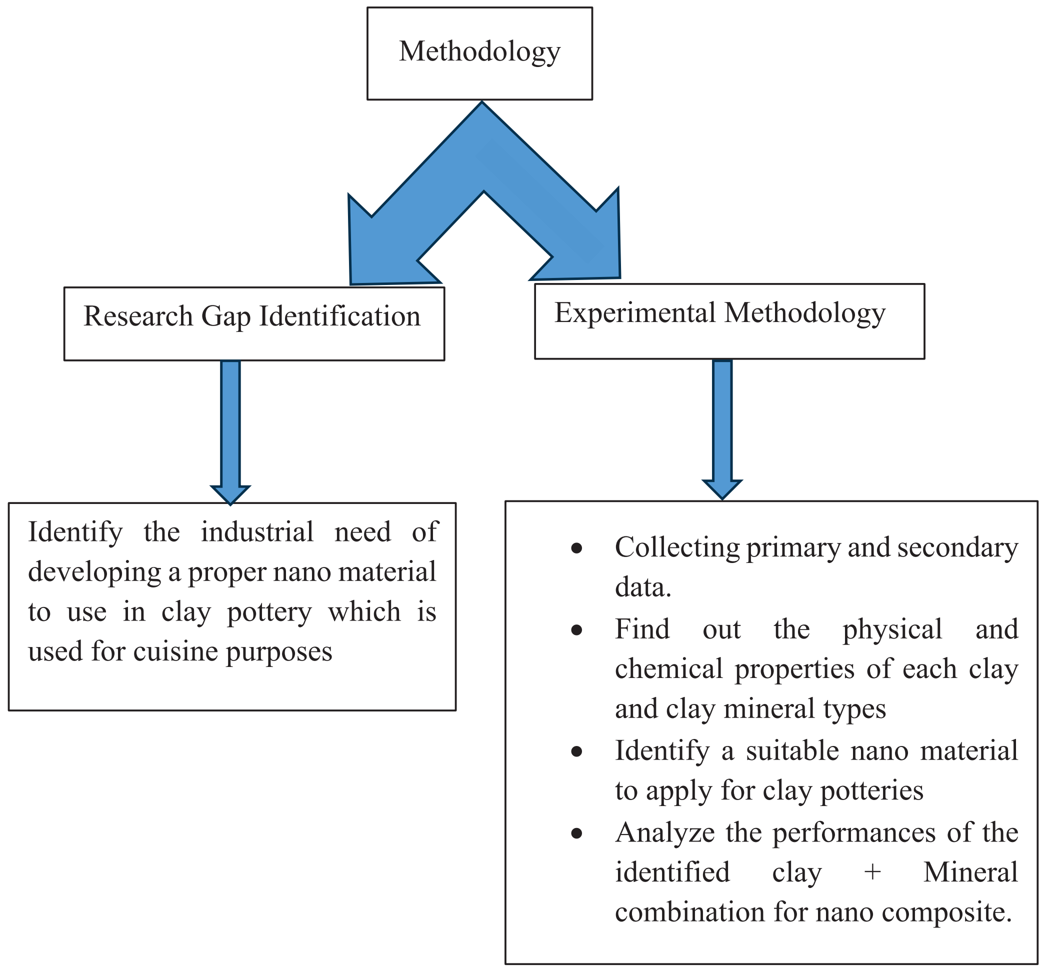


Figure 3.1: Complete research methodology

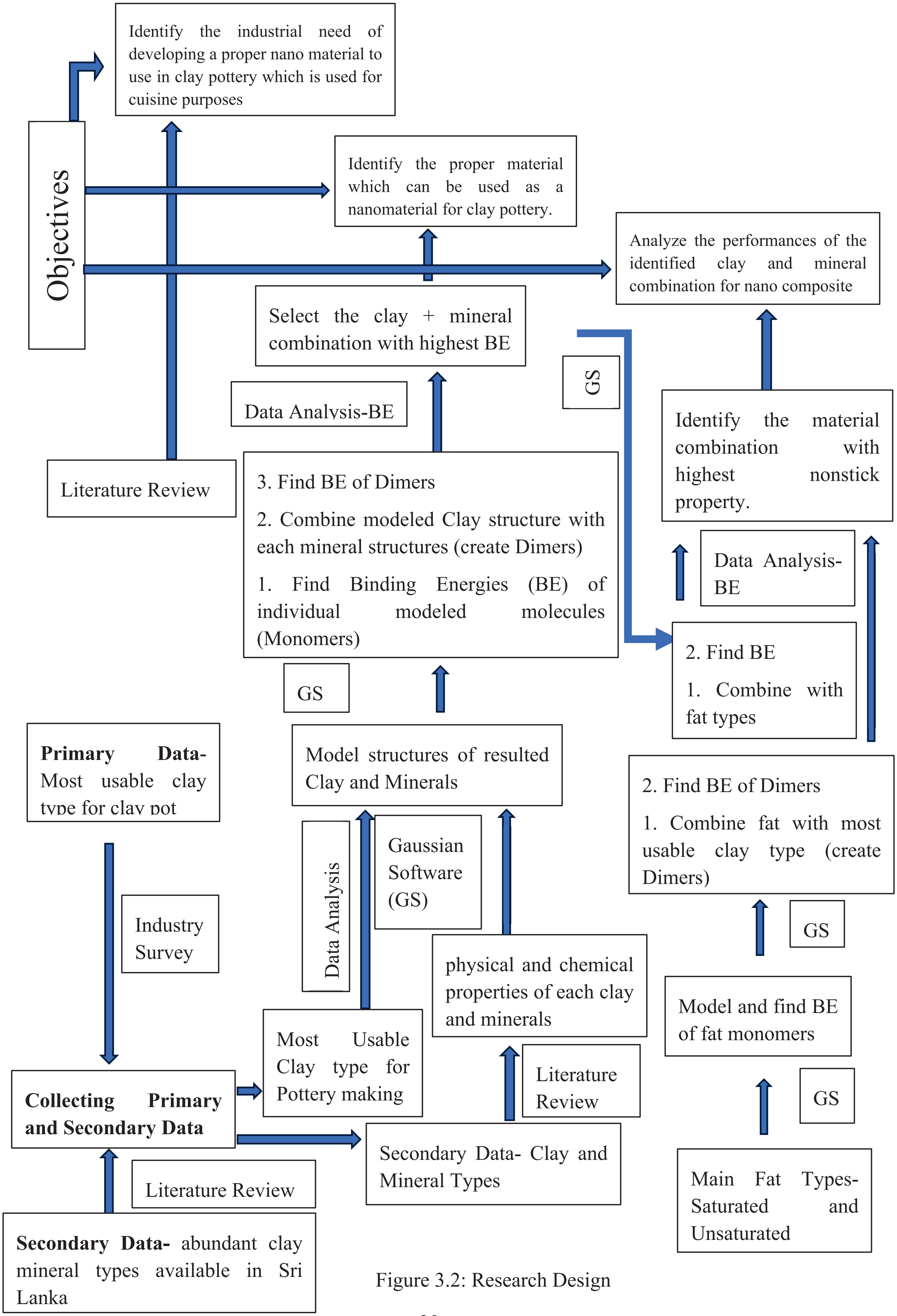


Figure 3.2: Research Design

3.2.1 Step-01: Collecting Primary and Secondary Data

The initial data accumulation was done through two ways, primary and secondary data collection. This was implemented to identify the main clay type use for cooking clay pottery making and abundant clay mineral types and non-metallic mineral types in Sri Lanka.

3.2.1.1 Primary Data Collection

The primary data collection was done through an industrial survey in pottery industry. The industry survey was carried out in Gampaha District by involving randomly selected 10 numbers of pottery making centers. They are situated in Weeragula, Minuwangoda, Meerigama and Kelaniya areas. Two of them are established by the Sri Lankan government as clay-based creations village and training centers at Weeragula and Kelaniya area. The remaining eight are medium-scale and small-scale domestic manufacturing centers situated in the above areas. This was conducted as a qualitative survey by having face-to-face interviews and telephone conversations with pottery makers and officers. A semi structured questionnaire including both open ended and closed ended questions was used as the data collection instrument. Then the gathered data were analyzed to find out the most usable clay type for pottery making, types of clayware, pottery making process and the gender participation in pottery making.

3.2.1.2 Secondary Data Collection

The literature survey was implemented to identify the abundant clay types, clay mineral and non-metallic mineral types available in Sri Lanka under the Literature Review (Chapter 2) part of the research. As Sri Lanka is a clay and mineral rich country this was implemented to find out the literature evidence for most suitable clay and mineral types which are used in the clay industry. The natural clay and clay mineral deposit areas and most usable industrial nonmetallic minerals were identified under the literature review part.

3.2.2 Step-02: Physical and Chemical Properties of Identified Clay Types and Minerals

The physical and chemical properties of the most usable clay type for pottery making, clay mineral types and industrial minerals which were identified under step 1, were investigated through the literature survey. These properties are chemical composition / formula, crystalline structures, chemical structure, appearance, color, mineral type and odor.

Though there are different types of clay types recognized according to literature review which are used for clayware, the most usable clay type was considered for further experiments identified through the industry survey. These properties were utilized in structuring the relevant clay and mineral types by using computational chemistry software (Gaussian) and they will be used in further development of this research in future activities in analyzing each mineral type during their physical experiments.

3.2.3 Step 03: Identify a Suitable Mineral Material to Apply for Clay Potteries as Nano Material

This consists of two experimental steps. Initially the models of identified most usable clay type through the industry survey and other identified minerals according to literature review were designed by using Gaussian software coming under computational chemistry. Secondly, finding the Binding Energies of molecules through the simulation process in GS and analyzing these values to identify the most suitable mineral type to collaborate with the identified clay type to make cooking potteries.

3.2.3.1 Use GS to Model Identified Clay and Mineral Structures

As per the literature review, the GS was used to model the molecules and for simulation process. Mainly the GS consists of three main interfaces which are Job Processing window, Gauss view interface, graphical interface. Gaussian 09 version and Gauss view 6 interface versions were used in this research as in Figure 3.3 (Gaussian.com, 2019).

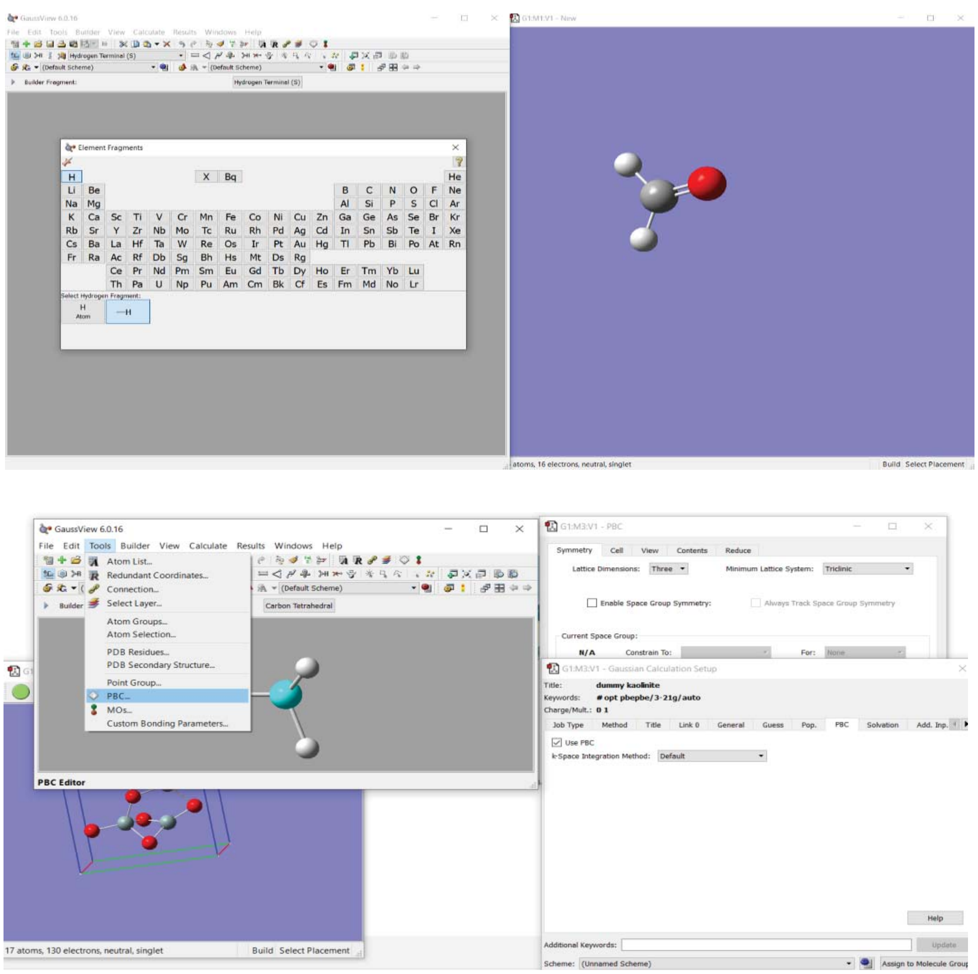


Figure 3.3: Modeling molecules using GS (Gaussian.com, 2019)

Initially each clay and mineral type were designed considered them as monomers. A monomer is a small molecule that can chemically bond with other similar or identical molecules to form a polymer. Monomers are the basic building blocks of polymers (Dhote et al., 2019). Monomers were designed using the relevant icons such as Element, R-Group Fragments, Periodic Boundary Conditions (PBC), modify Bond, Modify Angles and other necessary icons in Gauss view 6 interface and graphical interface by considering the referred literature regarding chemical composition / formula and crystalline /chemical structure in step 01.

3.2.3.2 Calculate Binding Energies of Monomers and Dimers by Simulation

The system binding energy was calculated by the simulation process using GS. As per the definition of the formula, the released energy when combining molecules is calculated by deducting the total energy of monomers from the total energy of the combined system. The auto calculated electronic energy values by the software are given in Atomic Unit and all the received values were converted to kilocalories per mole (kcal/mol). The formula below was used to calculate the binding energy of the system, and the interaction energy was avoided due to usage of binding energies for the research.

$$E_{(bind\ (mon\ A-\ mon\ B))} = E_{(opt\text{-}dimer\ AB)} - \left(E_{(opt\text{-}mon\ A)} + E_{(opt\text{-}mon\ B)}\right)$$

According to literature review the A and B letters show the separate monomers and E shows the Energy of the system (dimer). The combined system is called dimer, and a dimer is a molecule formed when two monomers (identical or different) chemically bond together (Holland et al., 2009)

There are important points to be concerned with calculating the BE of each system using GS.

- Do Geometry optimization and Frequency calculation (Opt+Freq) relevant molecules (Figure 3. 4)
- Use the Semiempirical theory option as the calculation method (Figure 3.5).
- Identify monomers to be combined (Atom Group Editor) (Figure 3.6)

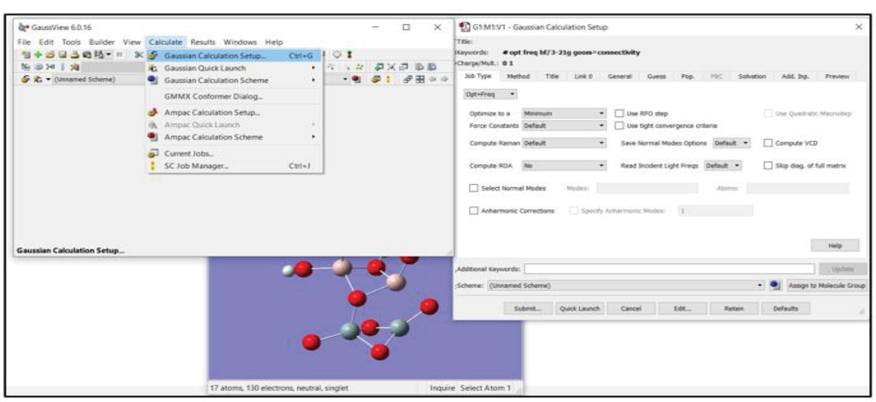


Figure 3.4: Geometry optimization and Frequency calculation (Opt + Freq) relevant molecules

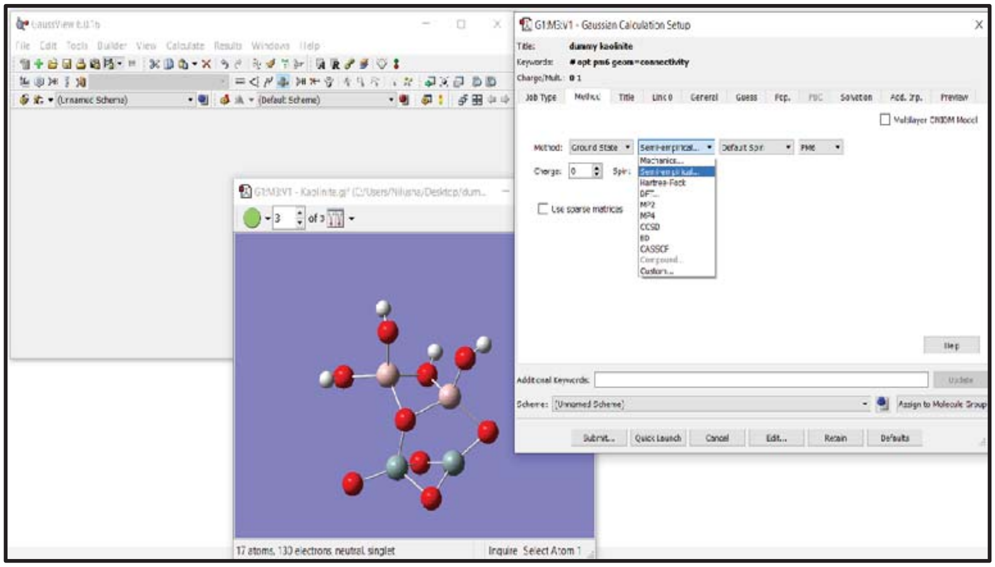


Figure 3.5: Semiempirical theory option as the calculation method

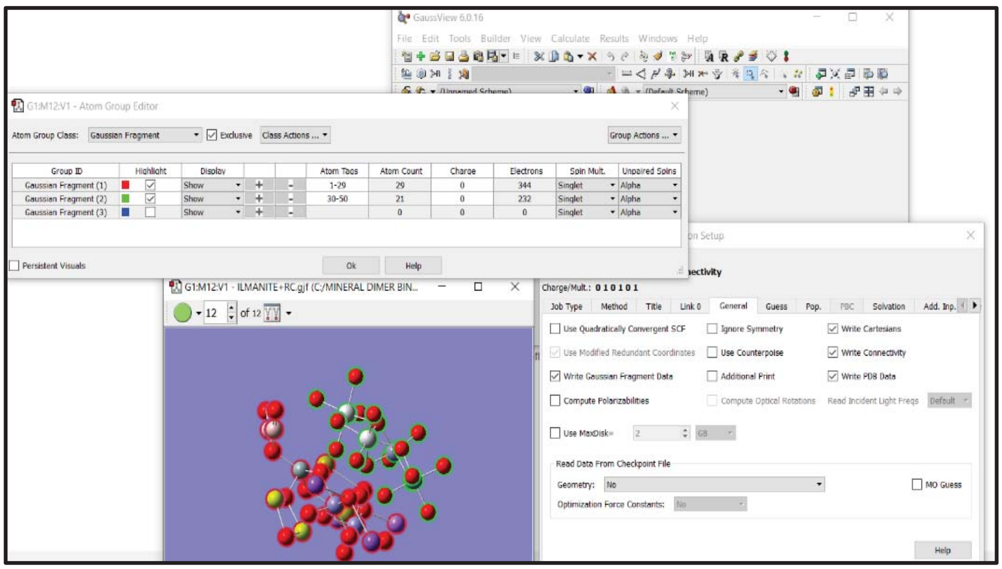


Figure 3.6: Identify monomers to be combined (Atom Group Editor)

Major steps of calculating BE are,

1. Calculate Energy of individual monomer
2. Combine each mineral with clay (Figure 3.7)
3. Calculate the total energy of the combined system
4. Deduct the accumulated energies of monomers from total energy of the system (dimer).

The combination order of clay and minerals to create dimers is shown in Figure 3.7. The identified clay type was considered as the monomer 01 in each reaction in the research. Each mineral type was considered as the monomer 02, to be combined with the monomer 01. The combined system which is consisted with both monomer 01 and 02 was considered as dimer.

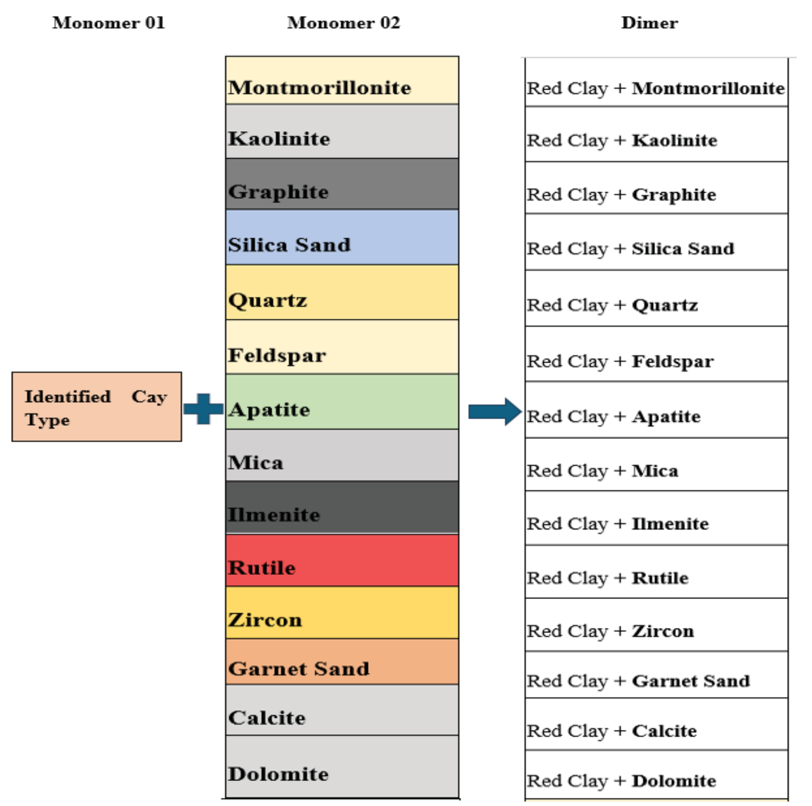


Figure 3.7: Clay and mineral combination

The energy values were stored in the Table 3.1 format for each clay and mineral combination

Table 3.1: Calculated energy value storing table

Binding Energy Calculation		
$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Monomer1+Monimer 2		
System	Electronic E (au)	Electronic E (kcal/mol)
Monomer 1		
Monomer 2		
Mixture (Combined system)		
Binding Energy		

Then the BEs for each clay + mineral combinations were analyzed to identify which combination has the highest negative valued binding energy to identify the best collaborative mineral material to the clay to use as a nano material. The (-) shows the exothermic reaction and this type of reaction exhibits the higher stability of the system. If the BE value will be positive (+) it shows the least stable system and endothermic reaction has occurred.

3.2.4 Step 04: Analyze the Performances of the Identified Clay + Mineral Combination for Nano Composite

Mainly the nonstick property of the identified clay and mineral combination was analyzed. According to the literature review, dietary fat/oil plays a major role in the human diet and there are two main types of saturated and unsaturated fats. Therefore, these fats were used to analyze the nonstick property of clay mineral combination by using GS. The steps of the analysis part as in Figure 3.8 are,

1. Model the fat/oil structures using GS and calculate the energies of each fat/oil type
2. Combine the clay with fat types separately and find the BEs
3. Combine the best clay and mineral combination with fat types separately and find the BEs
4. Store the Energy values in the table format (Table 3.1) for each reaction and compare the Bes.

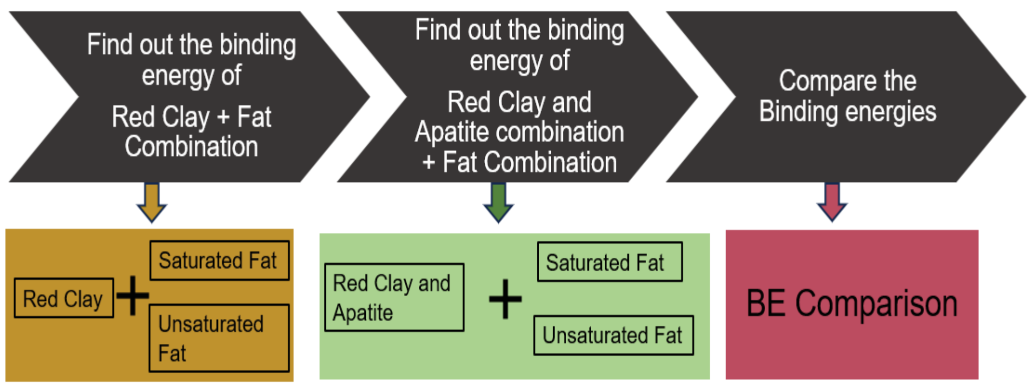


Figure 3.8: Analyzing nonstick property of identified clay + mineral combination

The analysis was done to identify which combination has the least BE whether it is between clay and fat/oil or clay + mineral mixture and fat/oil. The relevant combination with fat with the positive (+) BE value which is the most unstable system shows the higher nonstick property.

This was done for the general structures of saturated and unsaturated fats and for the oil types coming under each fat/oil type which are coconut oil and canola oil (vegetable oil).

3.3 Summary

This chapter consists of research methods towards achieving the research aim and objectives. They are, collecting primary and secondary data, literature on physical and chemical properties of identified clay types and minerals, identify suitable mineral material to apply for clay potteries as nano material by modeling identified clay and mineral structures and calculating binding energies of monomers and dimers by simulation using Gaussian software and finally analyzing the nonstick performances of the identified clay + mineral combination for nano composite.

The primary data collection was done through an industrial survey in Gampaha District. The secondary data collection was done through the literature review to find out the physical and chemical properties of identified clay types and minerals. Particularly the structures with chemical compositions were deliberated. These properties were contributed to modeling the clay and mineral types to calculate the BEs through the simulation by using GS. As the highest negative BE values show the more stable system of clay and minerals, the highest negative BEs value was considered to identify the best collaborative mineral material to combine with the clay. As the fat/oil is a major staple food type, it was used to analyze the nonstick property of recognized clay + mineral mixture through finding BEs by using GS. The nonstick property was analyzed with the lower negative BE value between the clay + mineral mixture and fat/oil type, which will be predicted that fat/oil type has non adhesive ability to the modified clay + mineral pottery making material.

CHAPTER 4

RESULTS AND DISSCUSSION

4.1 General

This chapter demonstrates the results and discussion of each methodological steps from the research gap identification to overall experimental results including the analyzed outcomes. Displaying relevant collected data and reporting the calculated and analyzed results were interpreted through the charts, graphs, texts, tables and statistical measures towards fulfilling of research objectives. Mainly the most usable clay type to make clay cooking pottery, the most appropriate mineral type to collaborate with clay type and the nonstick property of the identified clay and mineral combination, revealed through the various experimental steps in this chapter.

4.2 Research Gap Identification

The research gap identification was done in the introduction part based on the literature review and it addresses the objective identifying the industrial need of developing a proper nano material to use in clay pottery which is used for cuisine purposes. There are two main problems that are identified which are caused to generate the industrial need of developing proper nano material to use in clay pottery.

- Using of metal and nonstick metal cookware cause hygienic problems in human beings.
- Food stickiness to the inner surface of the clay pottery during cooking.

Therefore, recognizing of property improved material for making clay cooking pottery is a significant advanced movement for the development of pottery industry in Sri Lanka.

4.3 Experimental Results Overview

The experimental results overview consists of industrial survey results, identified abundant clay types, clay mineral and non-metallic mineral types in Sri Lanka, physical and chemical properties of identified clay type and minerals, binding energy analysis part to find out the most suitable mineral material to apply for clay potteries as nano material and to identify the nonstick performances of the identified clay + mineral combination for nano composite.

4.3.1 Step 01: Primary and Secondary Data

Most usable clay type for pottery making, industry type clay consumption, gender participation in pottery industry, industry type gender participation, types of clayware and pottery making process are identify through the industrial field survey under the primary data collection. Abundant clay types and industrial mineral types in Sri Lanka were shown through the secondary data based on the previous literature.

4.3.1.1 Industrial Survey Results

The industrial survey was mainly targeted on finding out the most usable clay type for pottery making, types of clayware, pottery making process and the gender participation in pottery industry.

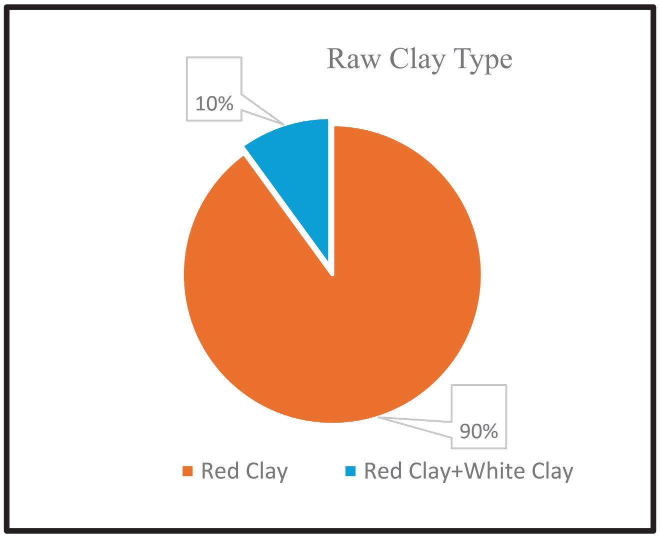


Figure 4.1: Most usable clay type for pottery making

According to the results of the industrial survey, Figure 4.1 shows 90% of respondents are using Red clay as the raw material in cooking pottery making. 10% of respondents are using a clay mix consisting of Red clay and white clay.

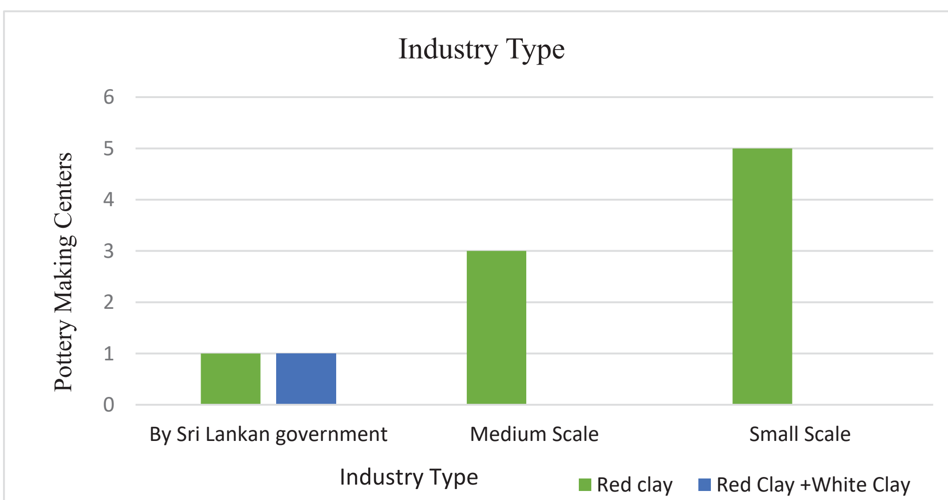


Figure 4.2: Industry type clay consumption

As shown in Figure 4.2, the medium-scale and small-scale domestic manufacturing centers use red clay for making cooking clay pots and only one government sponsored clay-based creations village and training center at Kelaniya uses both red clay and white clay mixture for pottery making and sometimes it depends on the supply of the white clay to the center. The majority of the pottery makers use red clay as raw material to make cooking pottery. Therefore, the most usable clay type for cooking pottery making is Red clay.

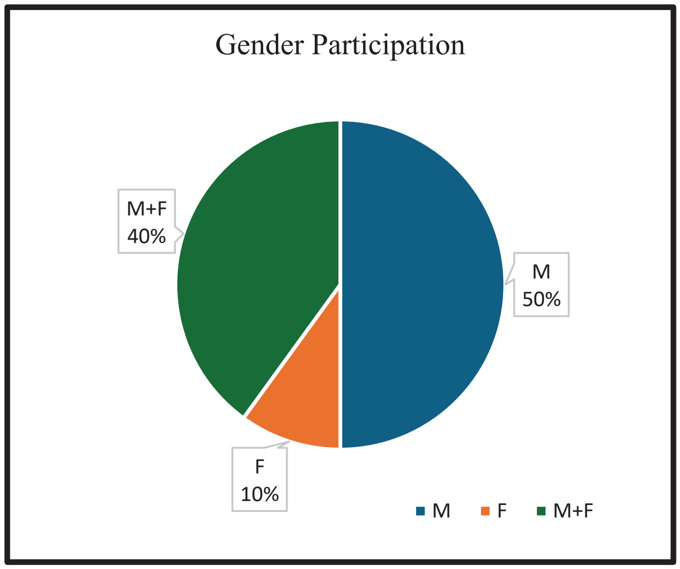


Figure 4.3: Gender participation in pottery industry

The gender participation in pottery industry is shown in Figure 4.3 describes that 50% of males are involving in pottery industry and the female contribution is 10%. Nevertheless 40% of both males and females are involving with pottery making.

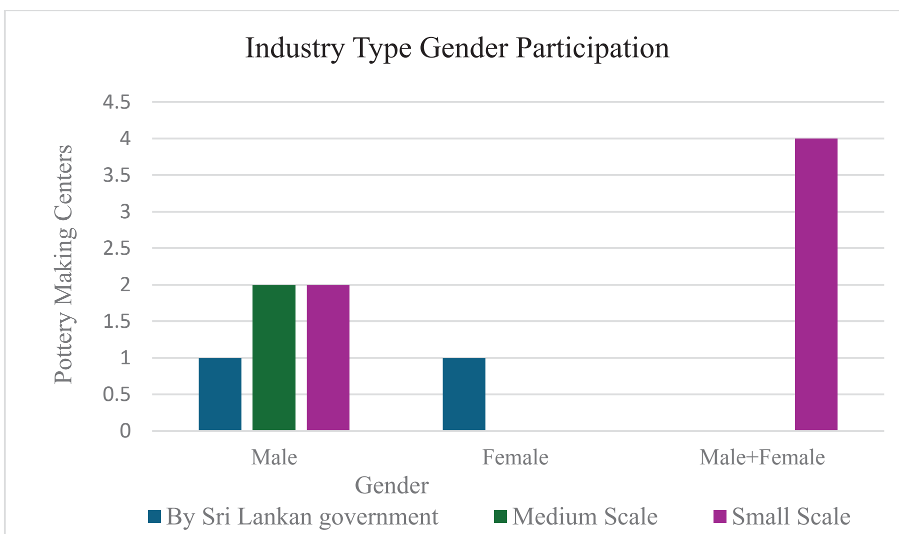


Figure 4.4: Industry type gender participation

The industry type gender participation shown in Figure 4.4 represents males' involvement in pottery industry is higher than both female and male + female involvements. However, both male and female are mostly involving in small scale domestic level pottery industry.

Types of clayware

The Different types of clayware which are manufactured in the visited clay centers are listed down in the Table 4.1 and the as per the conversation had with them, the quantity of these items depends on the requirements of the consumers. The cuisine clay potteries are made during the whole year and some non-cuisine clayware are seasonal products which are manufactured targeting the special cultural and religious occasions.

Table 4.1: Different types of clayware

Cuisine Clay Potteries	**Non-Cuisine Clayware**
Etili (use for cooking curries), Muttiya (use for boiling water, and cooking rice), Apalla (use for cooking food), Nambiliya (pot lid)	Milk pots, Clay lamps, clay stove, Terracotta, Guruleththu, Clay water kettle, Clay plates, Clay Bowl (mati paathraya), Mati koppaya, Flowerpots, Decoration items, Clay Handicrafts and etc…

Figure 4.5: Cuisine and non-cuisine clayware

Figure 4.6: Clayware making by using mould and "Sakaporuwa"

Pottery making process

As shown in the Figure 4.7 the general cooking pottery making process consists of the steps below as per the collected information from the pottery making centers.

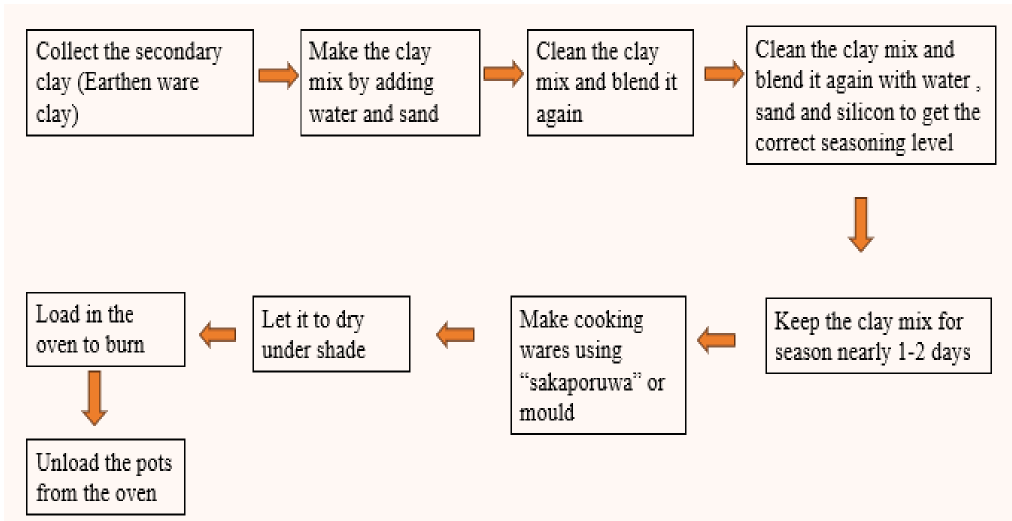


Figure 4.7: Cooking Pottery Making Process

Collecting the secondary clay (Red Clay/ Earthenware clay) is done by the clay suppliers who collect the relevant red clay from the clay sources. These pottery making centers are provided the Red clay from Negombo, Naththandiya and Panduwasnuwara in Sri Lanka.

Figure 4.8: Clay storing areas

Then the clay mixture is made by adding water and sand in necessary quantities while cleaning the blend by removing the unwanted parts such as stones. Next, the cleaned mixture is blended and cleaned repeatedly by adding more water, sand and silicon as necessary to create the optimum texture. Moreover less, the blended bulk is sent through a milling machine to ensure the maximum homogeneous texture and to cut the clay bulk into equal size clay cubes for user friendliness. Clay cubes are rested for 1-2 days for seasoning and cover with polythene.

Figure 4.9: Raw clay and initially cleaned clay

Figure 4.10: Clay mixing

Figure 4.11: Clay seasoning after mixing

Figure 4.12: Clay cubes partitioning

Then clay potteries are manufactured by using Sakaporuwa or mould. There are two types of Sakaporuwa which are manual and electric. All the clay centers use electric Sakaporuwa and 7 numbers of centers use moulds to make cooking potteries (Ethiliya) and milk pots. Other 3 numbers of small-scale pottery makers are not using moulds.

Figure 4.13: Clay pottery making by using “Sakaporuwa”

Figure 4.14: Clay pottery making by mould

Figure 4.15: Prepared pottery drying under shade before burning

Figure 4.16: New oven system

Figure 4.17: Old oven system

The potteries are dried under shade before loading them in the oven for some hours or days and then load them into the oven to burn. After proper burning time, the unloading of cured potteries is done from the oven and as the final stage allows them to cool.

Figure 4.18: Store clay pots in new oven system

Figure 4.19: Store clay pots in old oven system

Figure 4.20: Keeping burnt pots for cooling

Figure 4.21: Prepared clayware after oven process

4.3.1.2 Abundant Clay Types and Industrial Mineral Types in Sri Lanka

According to the literature review (Chapter 02) the abundant clay types which are used to make clayware and the industrial minerals are in Sri Lanka shown in Figure 4.22.

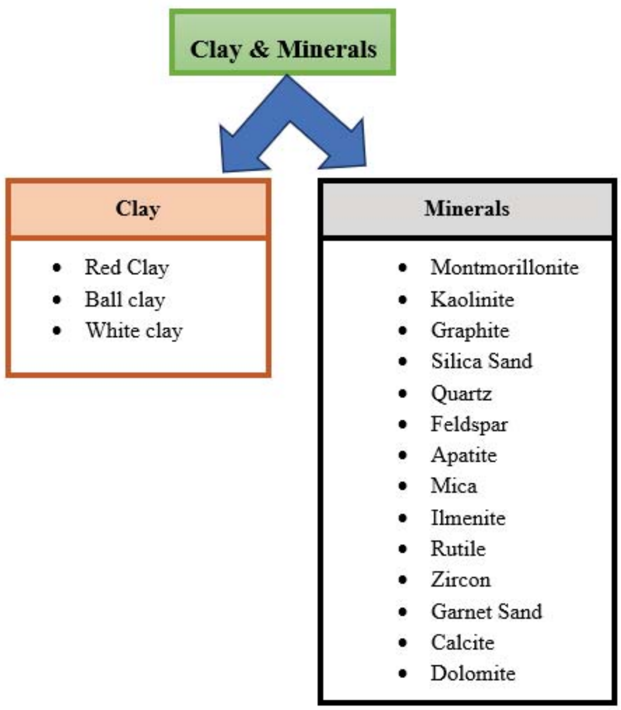


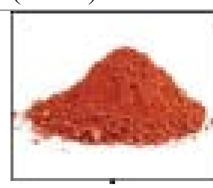
Figure 4.22: Clay types and industrial mineral types in Sri Lanka

According to step 01 the most usable clay type for cooking clay pottery is red clay. Therefore, only the Red clay is considered for future experiments in this research among other clay types.

4.3.2 Step 02: Physical and Chemical Properties of identified Clay Type and Minerals

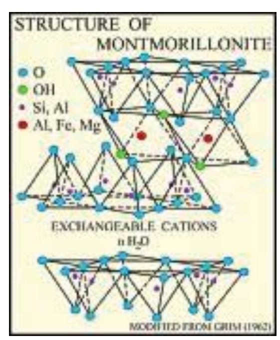
The relevant chemical and physical properties which are related to this study of identified red clay and industrial minerals are listed in each tables according to the literature survey. These properties are, chemical composition / formula, chemical structure, crystalline structure, appearance, color, mineral type and odor.

Table 4.2: The chemical and physical properties of Red Clay

Property	Value/ Description
Clay Type/Name	Red Clay
Chemical composition	Silica (SiO_2), Calcium Oxide (CaO), Iron (III) Oxide (Fe_2O_3) Magnesium Oxide (MgO), Aluminum Oxide (Al_2O_3), Potassium Oxide (K_2O), Sodium Oxide (Na_2O)
Appearance/Structure	
Color	Red-brown color

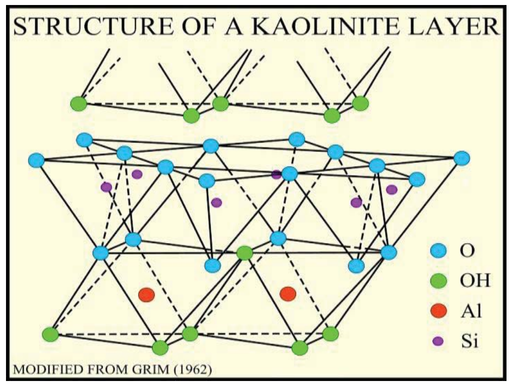
Source: (Samad et al., 2021)

Table 4.3: The chemical and physical properties of Montmorillonite

Property	Value/ Description
Mineral Name	Montmorillonite
Chemical composition/formula	$Al_2(OH)_2Si_4O_{10}$
Crystalline structure /system	
Color	Light Cream/Off white, Translucent

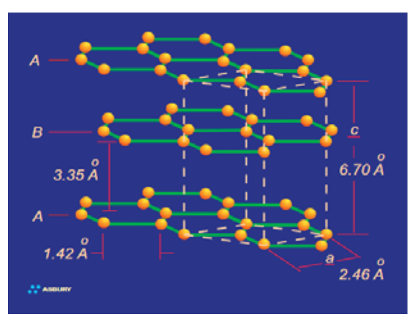
Source: (Nano Research Element, 2025; Poppe et al., 2001)

Table 4.4: The chemical and physical properties of Kaolinite

Property	Value/ Description
Mineral Name	Kaolinite
Chemical composition	$Al_2(OH)_4Si_2O_5$
Crystalline structure /system	Triclinic, Phyllosilicates (crystal class- Pedial) 
Color	Odorless white to yellowish or grayish powder
Odor	No odor

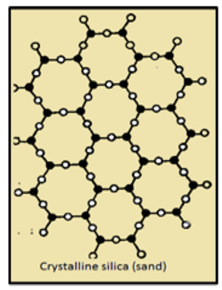
Source: (National Library of Medicine [NLM], 2024; Poppe et al., 2001)

Table 4.5: The chemical and physical properties of Graphite

Property	Value/ Description
Mineral Name	Graphite
Chemical Composition	Carbon atoms (Cn)
Crystalline Structure /system	Hexagonal 
Color	Black to steel grey
Mineral type	Native mineral

Source: (Matmatch, 2024; Asbury Carbons, 2025)

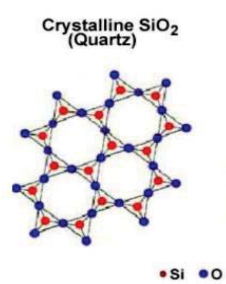
Table 4.6: The chemical and physical properties of Silica Sand

<table>
<tr><th>Property</th><th>Value/ Description</th></tr>
<tr><td>Mineral Name</td><td>Silica Sand</td></tr>
<tr><td>Chemical Composition</td><td>SiO_2, Al_2O_3, Fe_2O_3 – 0.02- (98.5% silica, as sand)</td></tr>
<tr><td>Cristal structure</td><td>Transparent crystals or amorphous powder



</td></tr>
<tr><td>Color</td><td>Blue, White crystal particles</td></tr>
<tr><td>Odor</td><td>Odorless</td></tr>
</table>

Source: (Wypych, 2021; ASDN, 2025)

Table 4.7: The chemical and physical properties of Quartz

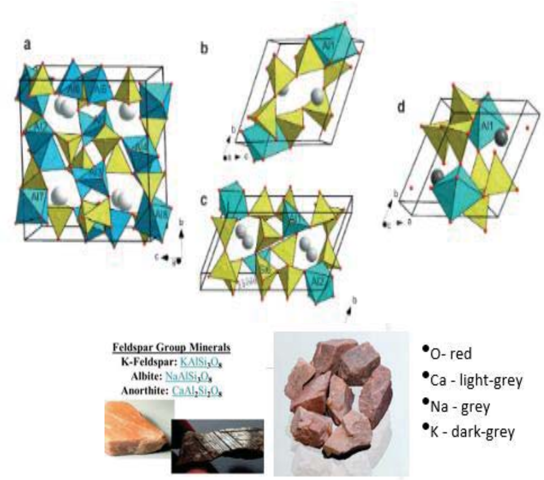
<table>
<tr><th>Property</th><th>Value/ Description</th></tr>
<tr><td>Mineral name</td><td>Quartz</td></tr>
<tr><td>Chemical composition/formula</td><td>SIO_2</td></tr>
<tr><td>Crystalline structure /system</td><td>• Crystalline form of silica.
• Mostly available silica type form of earth.
• Crystalline form of silica as granules, high purity silica-98-99.5%.




</td></tr>
<tr><td>Mineralogical analysis</td><td>• High percentage of quartz phase.
• High silica content and use as silica refractory brick.</td></tr>
<tr><td>Color</td><td>White</td></tr>
</table>

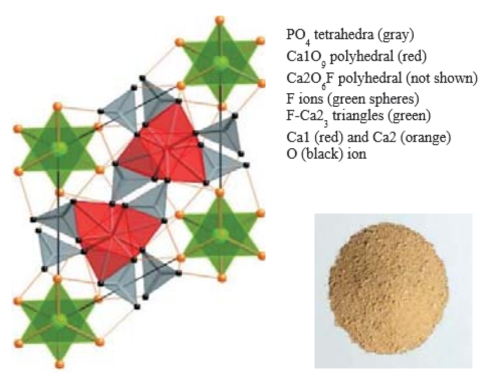
Source: (ChemicalBook, 2017; Paul et al., 2023)

Table 4.8: The chemical and physical properties of Feldspar

Property	**Value/ Description**
Mineral name	Feldspar
Chemical composition/ formula	(K_2O) $(SIO_2)_6(Al_2O_3)$
Crystalline structure /system	
Color	White, red

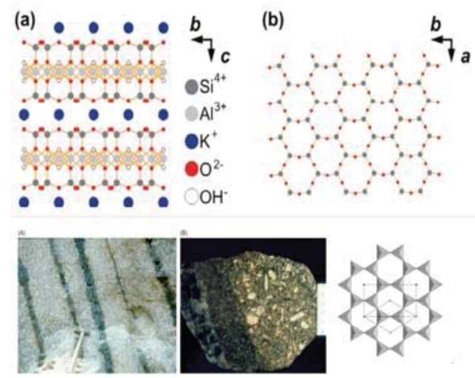
Source: (Wypych, 2021; Pakhomova et al., 2020)

Table 4.9: The chemical and physical properties of Apatite

Property	**Value/ Description**
Mineral name	Apatite
Chemical composition/ formula	$Ca_5(PO_4)$
Crystalline structure / system	Hexagonal
	
Color	White, Yellow, Green, Red, Blue.
Mohs scale- hardness	5

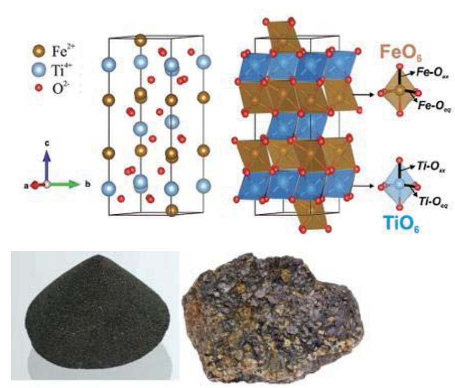
Source: (Apatite Mineral Data, 2014; Hazrah & Antao, 2022)

Table 4.10: The chemical and physical properties of Mica

Property	**Value/ Description**
Mineral name	Mica
Chemical Composition / Formula	$KAl_2(AlSi_3O_{10})(OH)_2$
Crystalline Structure /system	
Color	White to Green or Red to Black (Fine white powder)

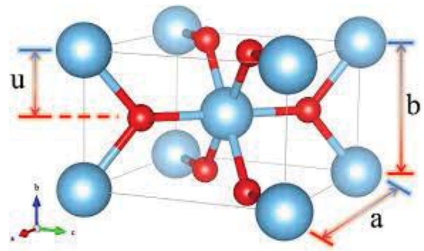
Source: (Zhang et al., 2019; Ostendorf et al., 2008)

Table 4.11: The chemical and physical properties of Ilmenite

Property	**Value/ Description**
Mineral name	Ilmenite
Chemical composition/ formula	$(Fe. TiO_3)$
Crystalline structure / system	Trigonal 
Color	Iron black, Black and Brittle

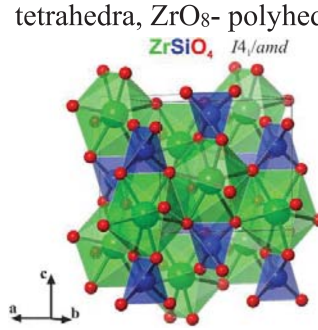
Source: (ChemicalBook, 2023; Ribeiro & de, 2014)

Table 4.12: The chemical and physical properties of Rutile

Property	**Value/ Description**
Mineral Name	Rutile
Chemical composition/Formula	TiO_2
Crystalline structure /system	Tetragonal  
Color	Red-brown to black

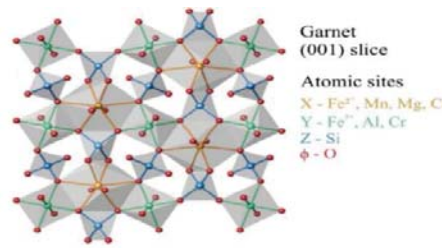
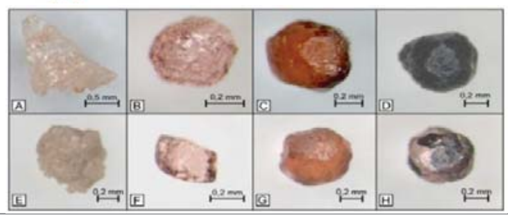
Source: (Shon et al., 2008; Azevedo et al., 2020)

Table 4.13: The chemical and physical properties of Zircon

Property	**Value/ Description**
Mineral name	Zircon
Chemical composition/ formula	$ZrSiO_4$
Crystalline structure /system	Gemstone (Avoided for further experiments due to High Cost) (SiO_4- tetrahedra, ZrO_8- polyhedral)  
Color	Gold Color. A gem (Yellow, Blue)

Source: (Burnham, 2018; Pina et al., 2018; Geology Science, 2018)

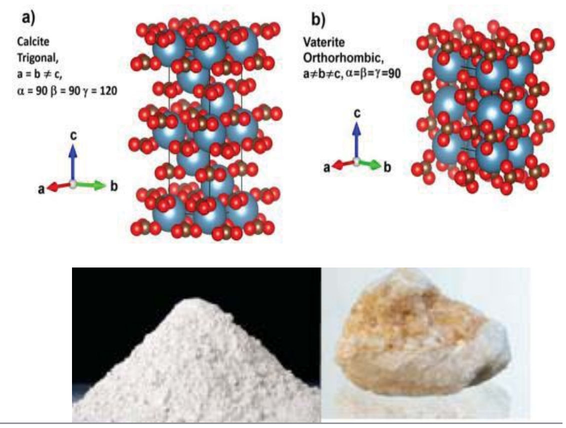
Table 4.14: The chemical and physical properties of Garnet Sand

Property	Value/ Description
Mineral Name	Garnet Sand
Chemical composition/ formula	Common Formula- $A_3B_2(SiO_4)_3$, A and B represent- Ca, Mg, Fe^{+2}, or Mn, Al, Cr, Fe^{+3} or Ti
Crystaline structure / system	Grain Shape- angular   
Color	Pink to red color
Odor	Odorless

Source: (Muttashar et al., 2017; Export Development Board Sri Lanka (2021); Grew et al., 2013)

Table 4.15: The chemical and physical properties of Calcite

Property	Value/ Description
Mineral name	Calcite
Chemical composition/ Formula	$CaCO_3$
Crystaline structure / system	• Trigonal or Hexagonal • Crystals are uncommon • Occurs as granular, masses, foliated or tabular in nature • Occurs as granular, masses, foliated or tabular in nature

	
Color	White or colorless with light shades of yellow, orange, blue, pink, red, brown, green, black and gray

Source: (Amar et al., 2012; Febrida et al., 2021)

Table 4.16: The chemical and physical properties of Dolomite

Property	**Value/ Description**
Mineral name	Dolomite
Chemical composition/ formula	(Ca, Mg) $(CO_3)_2$
Crystalline structure /system	Trigonal crystal system with rhombohedral habit (Powder or chip) 
Color	White, brown to orange

Source: (LookChem, 2018; Zucchini et al., 2014)

4.3.3 Step 03: Suitable Mineral Material to Apply for Clay Potteries as Nano Material

This is mainly consisting of two major steps that modeling of Red clay and identified minerals and calculating the Binding Energies of each monomer and dimer through simulation in GS. Finally, BEs of each system (dimers) were analyzed to find out the most suitable mineral.

4.3.3.1 Modeled Red Clay and Minerals Structures Using Gaussian Software

According to Table 4.2, the Red clay is comprising of different types of compounds and the total structure as a clay was not found out through the literature review. According to the ingredient compounds the structure of Red clay was buildup through GS. Nevertheless, the structures of each mineral were modeled by using the information in step-02 in Gaussian. Modeled structures are shown below.

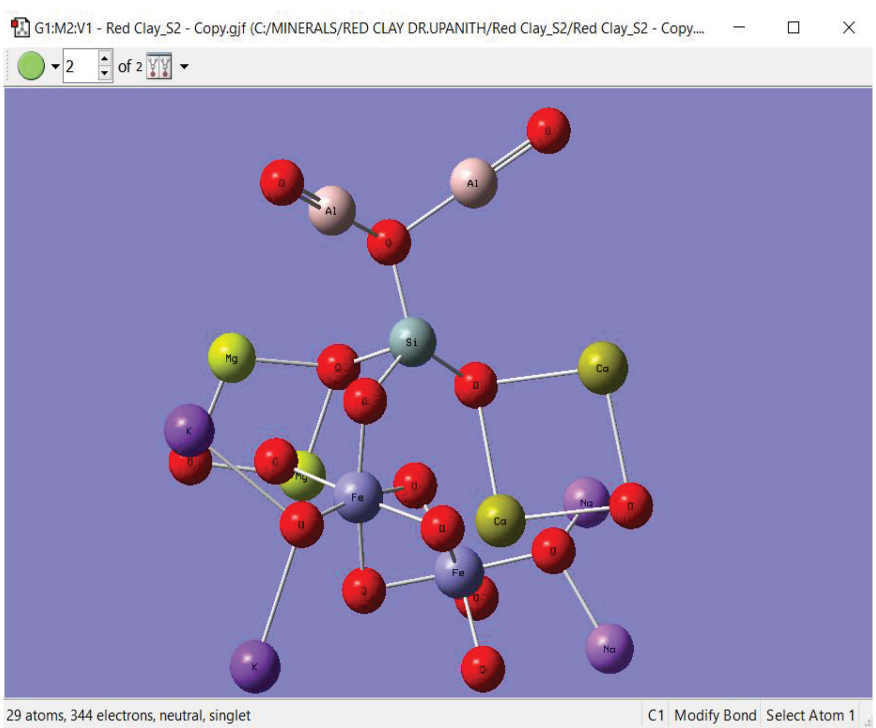


Figure 4.23: Modeled Red Clay using GS

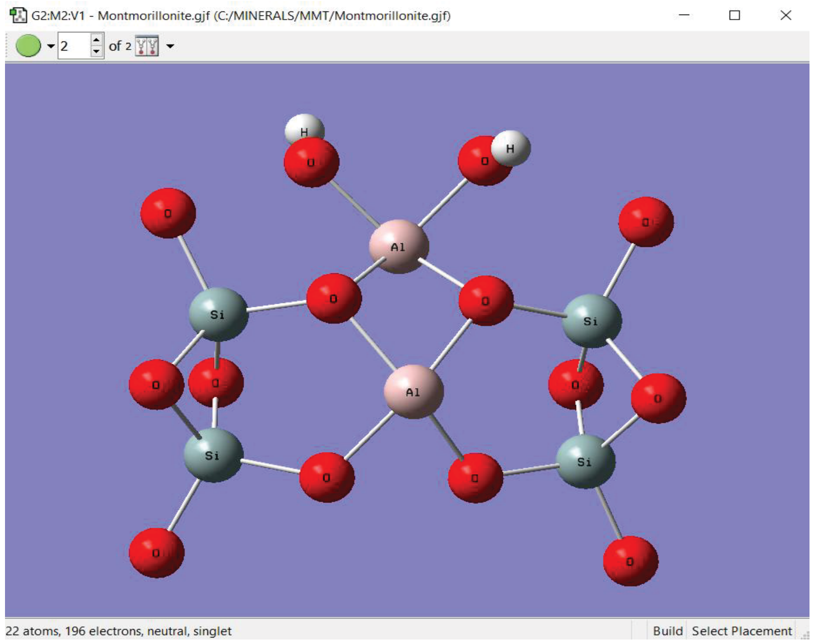


Figure 4.24: Modeled Montmorillonite using GS

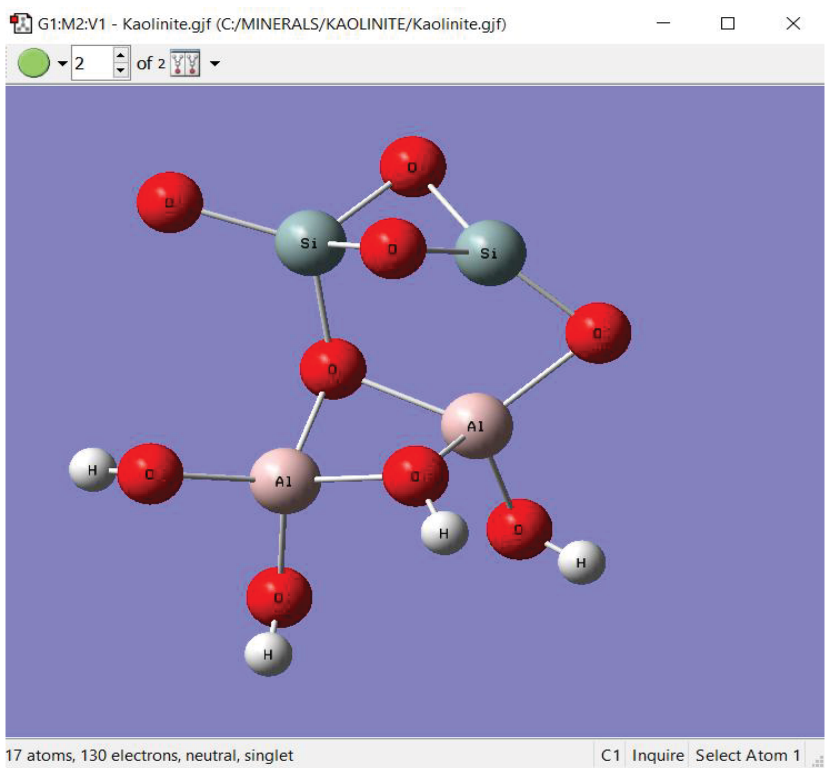


Figure 4.25: Modeled Kaolinite using GS

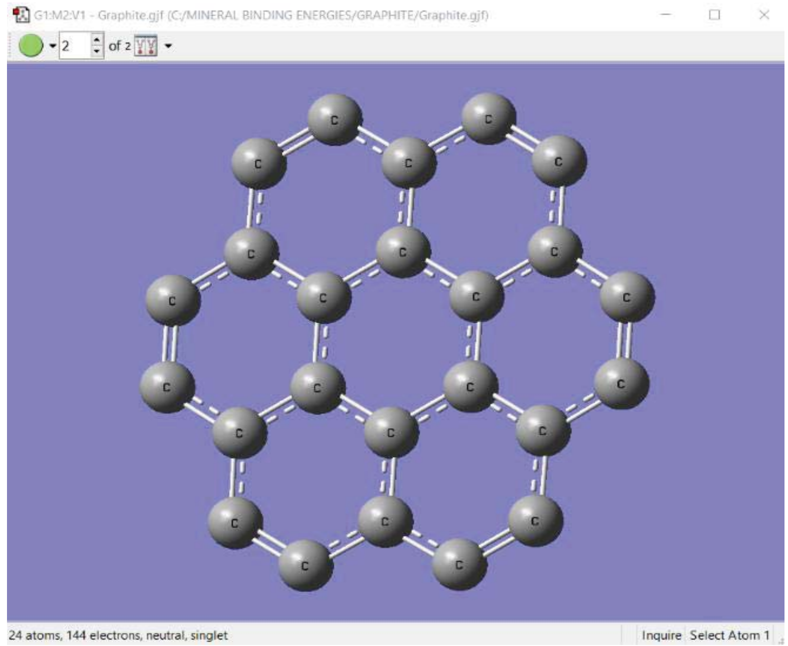


Figure 4.26: Modeled Graphite using GS

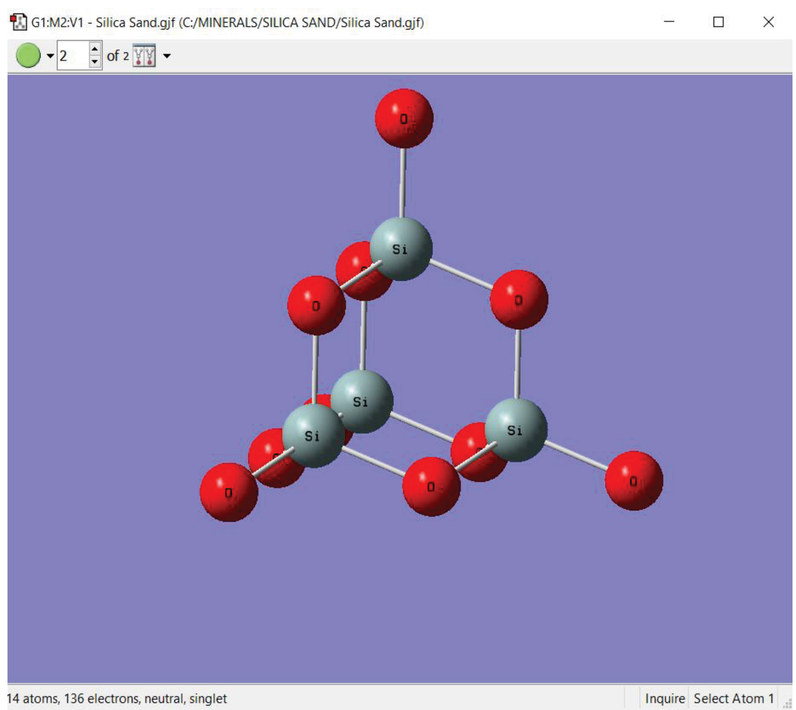


Figure 4.27: Modeled Silica Sand using GS

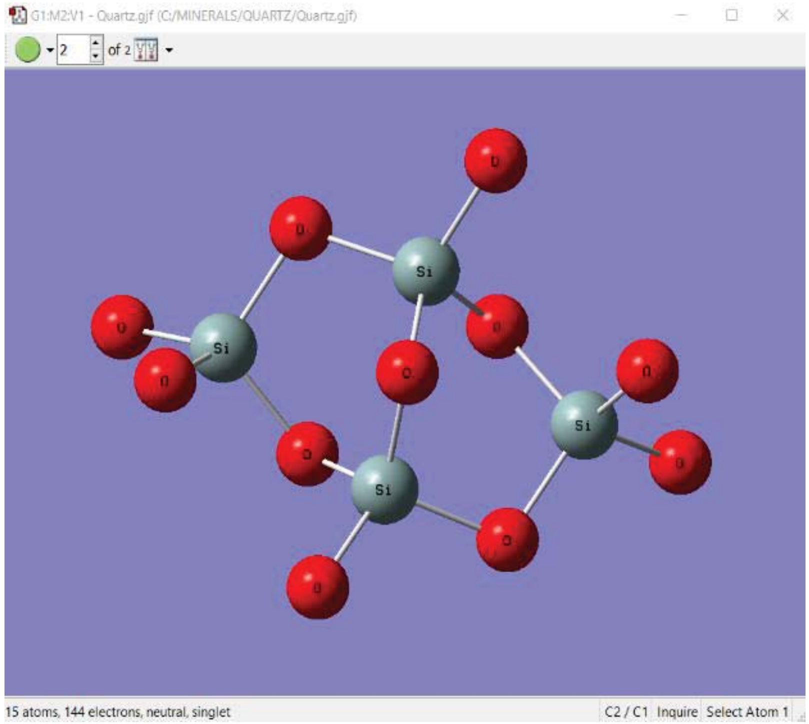


Figure 4.28: Modeled Quartz using GS

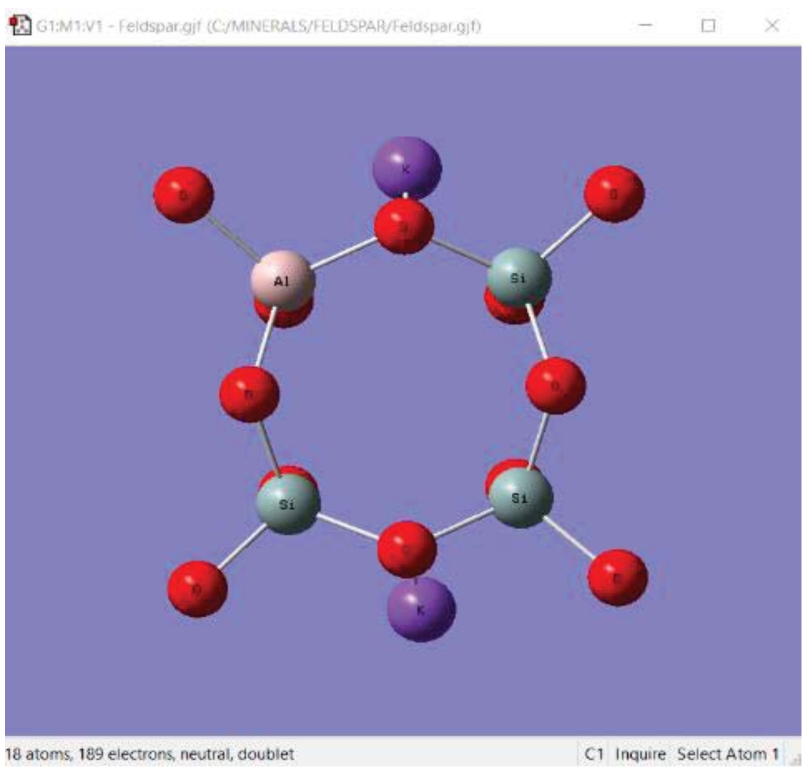


Figure 4.29: Modeled Feldspar using GS

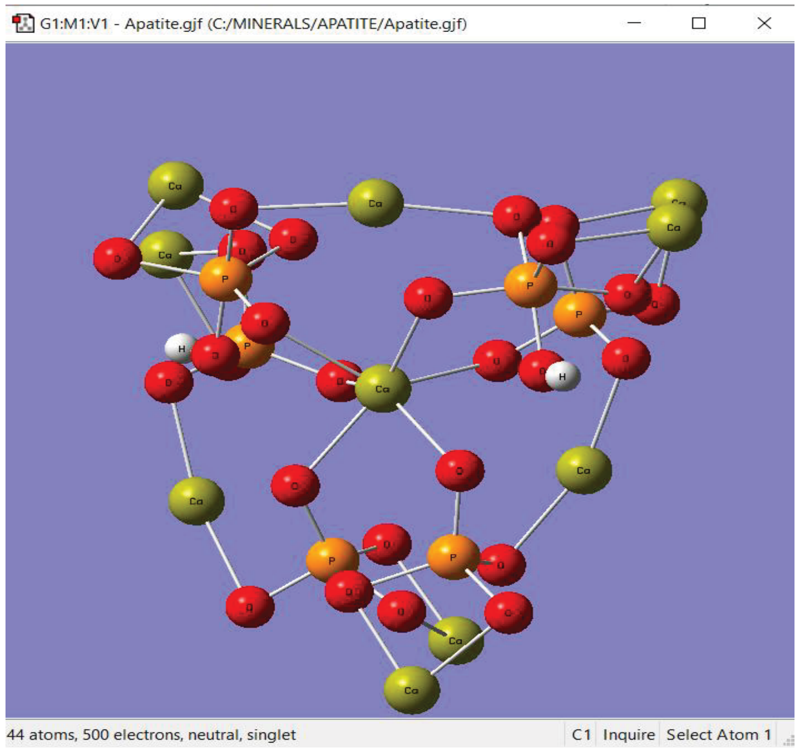


Figure 4.30: Modeled Apatite using GS

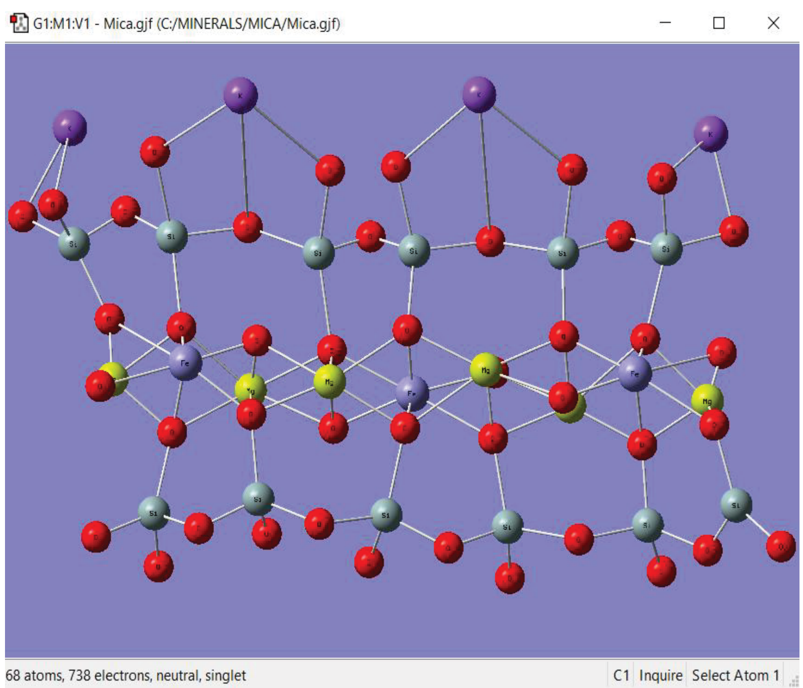


Figure 4.31: Modeled Mica using GS

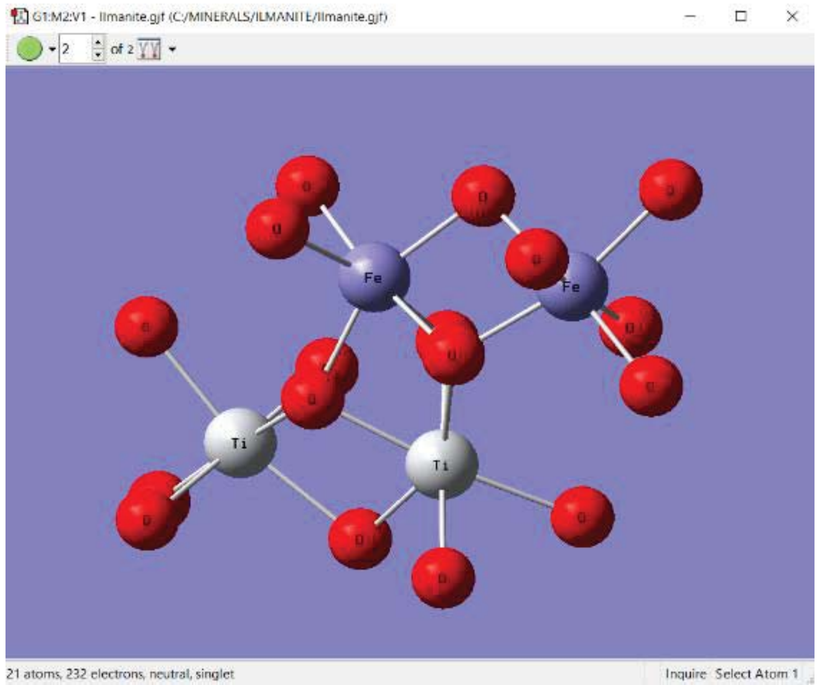


Figure 4.32: Modeled Ilmenite using GS

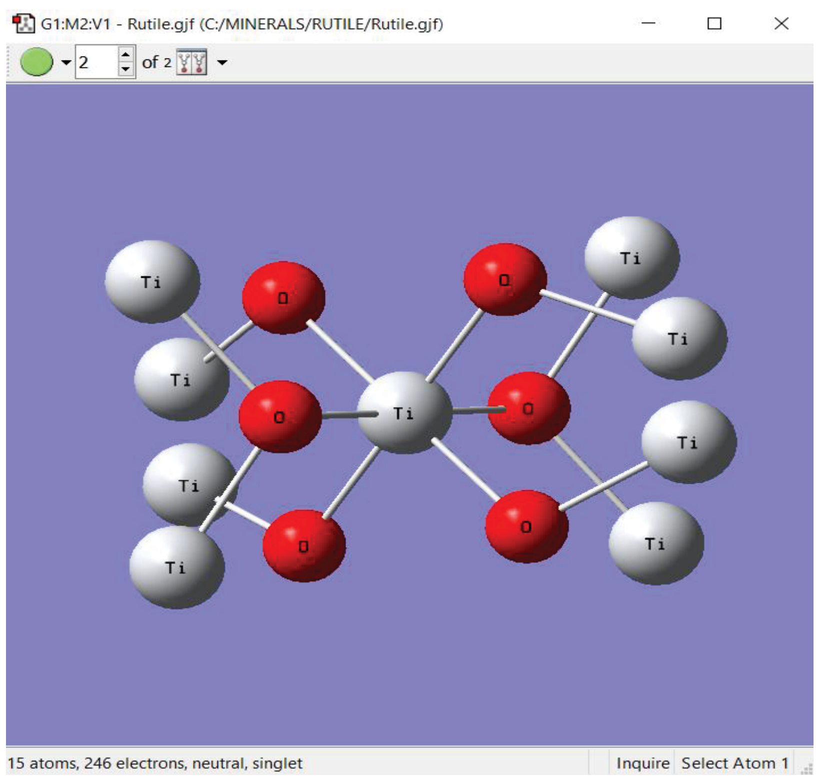


Figure 4.33: Modeled Rutile using GS

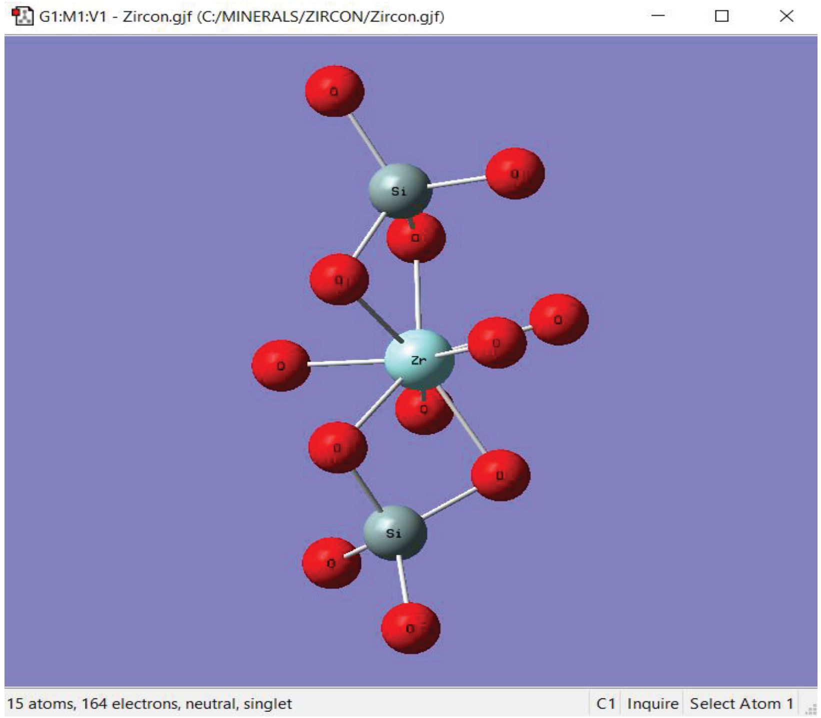


Figure 4.34: Modeled Zircon using GS

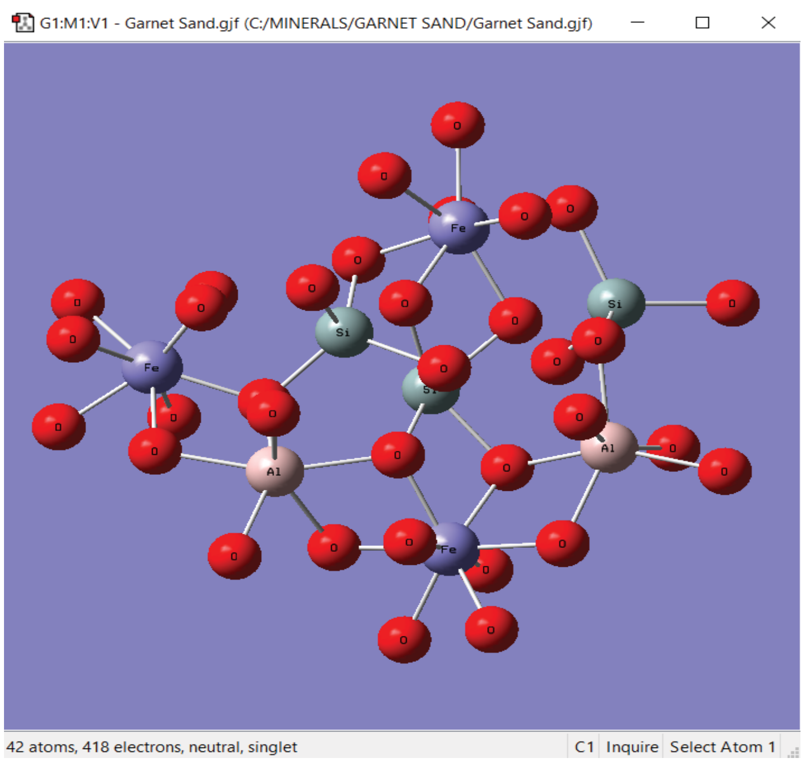


Figure 4.35: Modeled Garnet Sand using GS

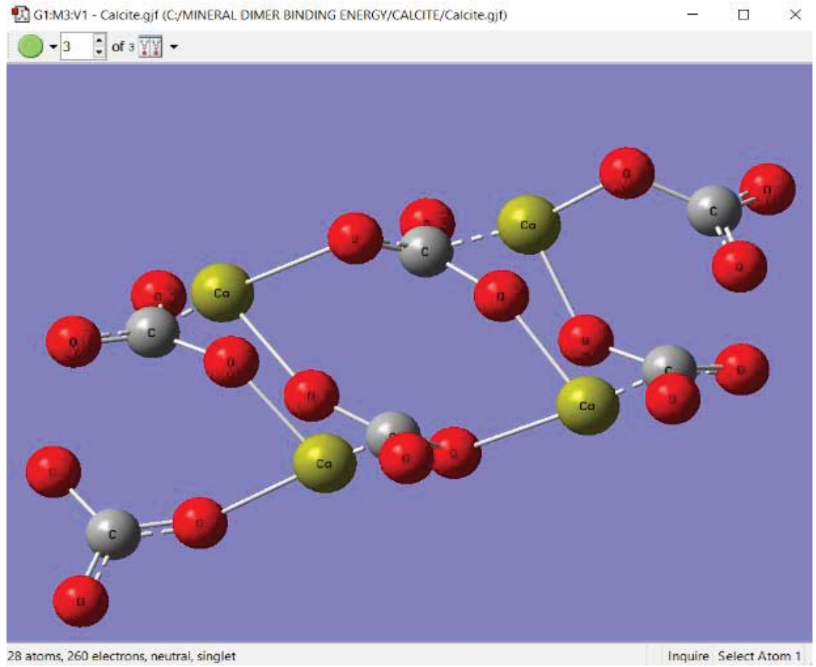


Figure 4.36: Modeled Calcite using GS

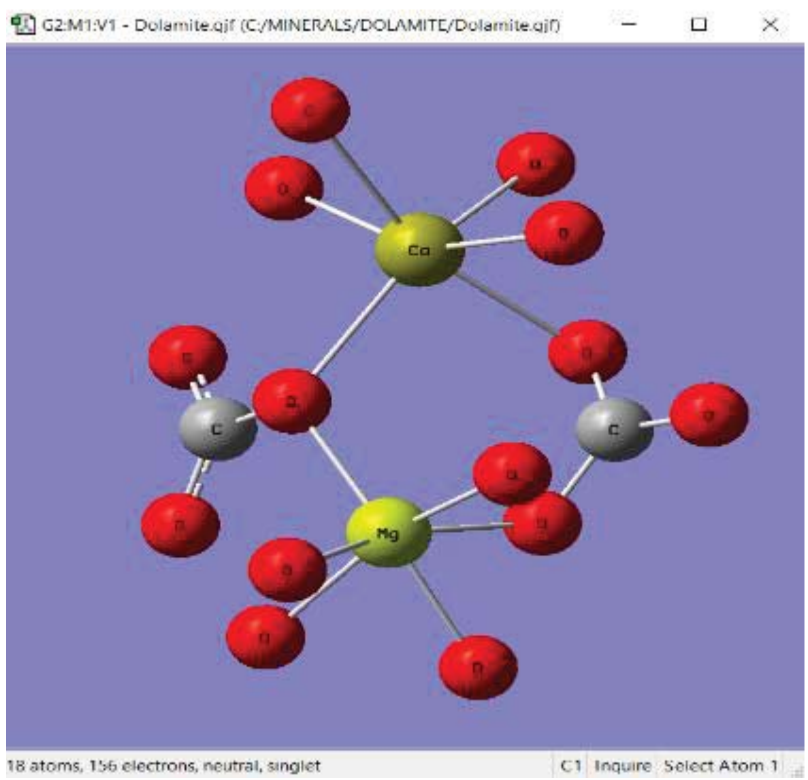


Figure 4.37: Modeled Dolomite using GS

4.3.3.2 Calculated Binding Energies of Monomers and Dimers Through Simulation and Binding Energy Analysis

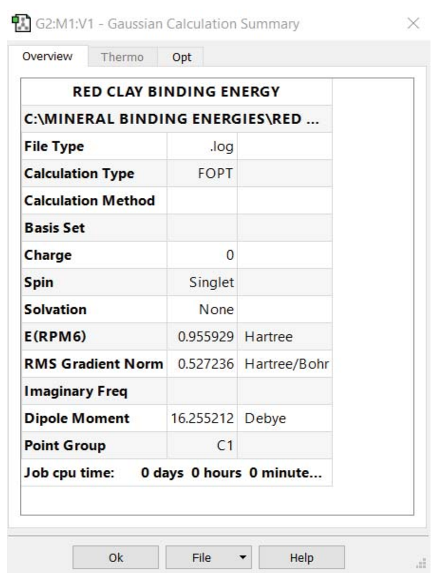
Calculated BEs of Monomers and Dimers Through Simulation

The energies of the above modeled Red clay and mineral structures (monomers) were calculated by simulation process through GS. Then the energies of each dimer which were generated by combining modeled Red clay with each mineral individually, were calculated by simulation through the GS.

These relevant energies are shown in below "Gaussian Calculation Summery" figures which were generated at the end of the simulation/ calculations for each monomer and dimer in GS. The sample "Gaussian Calculation Summery" tables are shown for Red clay and Montmorillonite combination and all other energy calculations were done in the same manner for each Red clay and mineral combination separately. The relevant BE value is exhibited in the raw, E(RPM6) in the Gaussian Calculation Summery table. The BE calculations which were done according to the mentioned formula for each Red clay and mineral combination is shown in separate tables.

The relevant energy values are given in "Hartree" unit in the raw E(RPM6) and it is the unit of energy which is Atomic Unit (au) which is represented in molecular orbital calculations. Moreover, the energy results of computations under Semiempirical method are recorded in Hartree (National Institute of Standards and Technology, 2022). For the convenience of further experimental works, the unit conversion from Hartree to kilocalories per mol (kcal/mol) is an important activity when using it in molecular calculations. Therefore, the final calculated BE values in Atomic Unit (Hartree) are converted to kcal/mol by multiplying the atomic unit values by 627.5 in this research.

Red Clay



RED CLAY BINDING ENERGY		
C:\MINERAL BINDING ENERGIES\RED ...		
File Type	.log	
Calculation Type	FOPT	
Calculation Method		
Basis Set		
Charge	0	
Spin	Singlet	
Solvation	None	
E(RPM6)	0.955929	Hartree
RMS Gradient Norm	0.527236	Hartree/Bohr
Imaginary Freq		
Dipole Moment	16.255212	Debye
Point Group	C1	
Job cpu time:	0 days 0 hours	0 minute...

Figure 4.38: Gaussian Calculation Summery for Red Clay

Red Clay and Montmorillonite

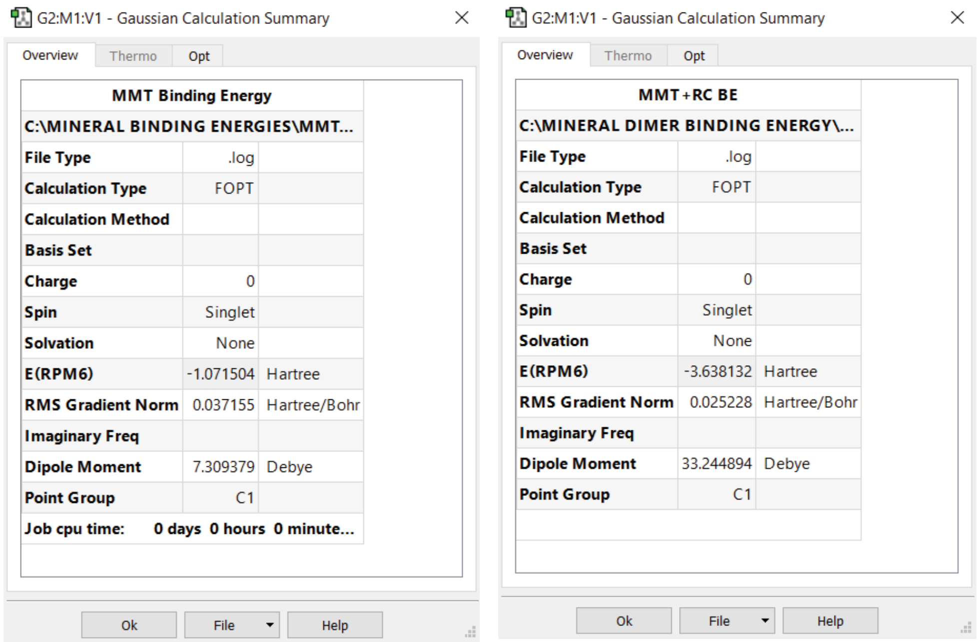


Figure 4.39: Gaussian Calculation Summery for Montmorillonite and for Red Clay and Montmorillonite System

Table 4.17: BE Calculation for Red Clay and Montmorillonite Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Montmorillonite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
MMT	-1.071504	
Mixture	-3.638132	
Binding Energy	-3.522557	-2210.404518

Red Clay and Kaolinite

Table 4.18: BE Calculation for Red Clay and Kaolinite Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Kaolinite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Kaolinite	-1.2153	
Mixture	-2.74491	
Binding Energy	-2.485539	-1559.675723

Red Clay and Graphite

Table 4.19: BE Calculation for Red Clay and Graphite Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Graphite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Graphite	1.110617	
Mixture	-1.097829	
Binding Energy	-3.164375	-1985.645313

Red Clay and Silica Sand

Table 4.20: BE Calculation for Red Clay and Silica Sand Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Silica Sand		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Silica Sand	-0.59582	
Mixture	-3.31869	
Binding Energy	-3.678799	-2308.446373

Red Clay and Quartz

Table 4.21: BE Calculation for Red Clay and Quartz Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Quartz		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Quartz	-0.636805	
Mixture	-3.621283	
Binding Energy	-3.940407	-2472.605393

Red Clay and Feldspar

Table 4.22: BE Calculation for Red Clay and Feldspar Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Feldspar		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Feldspar	0.303712	
Mixture	1.66058	
Binding Energy	0.400939	251.5892225

Red Clay and Apatite

Table 4.23: BE Calculation for Red Clay and Apatite Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Apatite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Apatite	-2.598435	
Mixture	-6.705931	
Binding Energy	-5.063425	-3177.299188

Red Clay and Mica

Table 4.24: BE Calculation for Red Clay and Mica Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Mica		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Mica	0.788721	
Mixture	-1.233375	
Binding Energy	-2.978025	-1868.710688

Red Clay and Ilmenite

Table 4.25: BE Calculation for Red Clay and Ilmenite Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Ilmenite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Ilmenite	0.734166	
Mixture	3.499009	
Binding Energy	1.808914	1135.093535

Red Clay and Rutile

Table 4.26: BE Calculation for Red Clay and Rutile Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Rutile		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Rutile	0.622766	
Mixture	-2.567815	
Binding Energy	-4.14651	-2601.935025

Red Clay and Zircon (Gemstone)

Table 4.27: BE Calculation for Red Clay and Zircon Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Zircon		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Zircon	-0.441609	
Mixture	-2.221052	
Binding Energy	-2.735372	-1716.44593

Red Clay and Garnet Sand

Table 4.28: BE Calculation for Red Clay and Garnet Sand Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Garnet Sand		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Garnet Sand	1.015729	
Mixture	2.727684	
Binding Energy	0.756026	474.406315

Red Clay and Calcite

Table 4.29: BE Calculation for Red Clay and Calcite Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Calcite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Calcite	-0.68596	
Mixture	-1.567384	
Binding Energy	-1.837353	-1152.939008

Red Clay and Dolomite

Table 4.30: BE Calculation for Red Clay and Dolomite Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Dolomite		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Dolomite	1.315221	
Mixture	2.318326	
Binding Energy	0.047176	29.60294

Binding Energy Analysis

Each finale BEs of red clay and mineral combinations are shown below Table 4.31 to compare the BEs of each system. They consist of both negative and positive BE values and the kcal/mol values are rounded to the nearest whole number for easy reference. According to the literature review (Chapter 2) the (-) BE values represent the exothermic reactions which are form stable product by releasing the energy to the outer environment and the (+) BE values show the endothermic reactions by forming an unstable product.

Therefore, the stable product contains higher adhesion ability between the included compounds. In another words, the products which are generated through exothermic reactions are more stable and they have strong interactions between molecules. According to Table 4.31 the BEs of the combinations of Red clay and Montmorillonite, Red clay and Kaolinite, Red clay and Graphite, Red clay and Silica Sand, Red clay and Quartz, Red clay and Apatite, Red clay and Mica, Red clay and Rutile, Red clay and Zircon then Red clay and Calcite are with negative BE values.

Table 4.31: BEs Comparison of Red Clay and Mineral Combinations

Mineral	**Montmorillonite**	**Kaolinite**	**Graphite**	**Silica Sand**	**Quartz**	**Feldspar**	**Apatite**	**Mica**	**Ilmenite**	**Rutile**	**Zircon**	**Garnet Sand**	**Calcite**	**Dolomite**
	Red Clay													
BE (au)	-3.52256	-2.48554	-3.16438	-3.6788	-3.94041	0.400939	-5.06343	-2.97803	1.808914	-4.14651	-2.73537	0.756026	-1.83735	0.047176
BE (kcal/mol)	-2210	-1560	-1986	-2308	-2473	252	-3177	-1869	1135	-2602	-1716	474	-1153	30

These values demonstrate that each single combination has strong intermolecular interactions between the Red clay and the relevant minerals. Hence, they have more stable systems. The sequence of system stability depends on the BE value. The higher (-) BE value represents the more stable clay + mineral system.

Meanwhile Red clay and Feldspar, Red clay and Ilmenite, Red clay and Garnet Sand and then Red clay and Dolomite combinations have (+) BEs. These values demonstrate that each single combination has weak intermolecular interactions between the Red clay and the relevant minerals. Meanwhile they have low stable systems. The sequence of system stability depends on the BE value. The higher (+) BE value represents the lowest stable clay + mineral system.

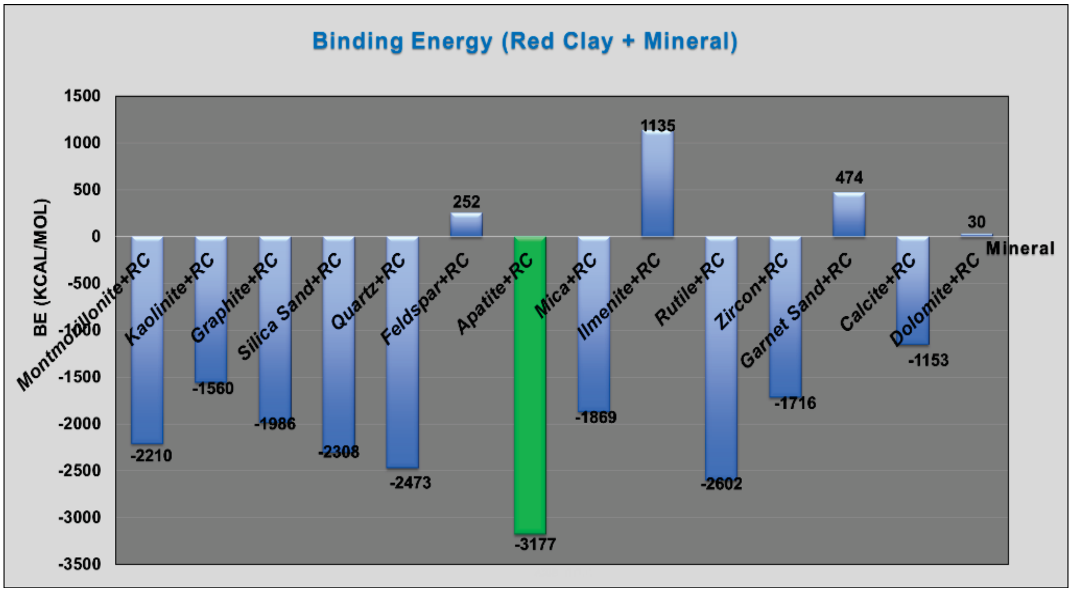


Figure 4.40: Red Clay + Material combination with Highest (-) BE

According to the BEs in Table 4.31, Figure 4.40 shows a graphical display of negative and positive BE value levels. According to that the Red clay and Apatite combination has the highest (-) BE value -3177 kcal/mol. Therefore, it has the steadiest system with the strongest intermolecular interaction performing highest binding ability between Red clay and Apatite. Thus, the Apatite mineral has the highest ability to combine with Red clay with strong adhesion capability.

When considering the importance of applying nanotechnology, the particle size of a material significantly influences its binding energy, with an inverse relationship between the two materials. As particle size decreases, the binding energy of the system increases. Consequently, utilizing nanoparticles results in higher binding energy due to stronger intermolecular forces, leading to a more stable system.

Hence the preparation of nano material using Apatite and applying it for making a compound with Red clay is more important to enhance the binding energy value between the Red clay and Apatite combination by creating more steady system.

4.3.4 Step 04: Nonstick Performances of the Identified Clay + Mineral Combination for Nano Composite

Step 04 consists of four main stages which are designed models of fat/oil (saturated, unsaturated, coconut oil and vegetable oil), calculated BEs of Red clay and fat/oil (saturated, unsaturated, coconut oil and vegetable oil) combinations, calculated BEs of Red clay + Apatite mixture with fat/oil combinations and finally the nonstick property performances through binding energy analysis.

4.3.4.1 Designed Models of Fat/Oil (Saturated Fat, Unsaturated Fat, Coconut Oil and Vegetable Oil)

As the fat/oil is an important part of the humans' diets, they are used in preparing the foods and some foods consist with higher percentage of fat/oil such as different kinds of edible oils, butter, nuts and other relevant foods. In finding the nonstick property performances of clay pottery making materials which were identified in Step 03, the models of relevant fat/oil structures which are used, shown under this section.

Initially the structures were modeled for saturated and unsaturated fat/oil structures. They are saturated, unsaturated, coconut oil and vegetable oil as below mentioned figures (Figure 4.41, 4.42, 4.43, 4.44). Lauric fatty acid ($CH_3(CH_2)_{10}COOH$) (Seneviratne & Jayathilaka, 2016) was modeled under general saturated fat category and Alpha- Linolenic acid ($C_{18}H_{30}O_2$) (Akay et al., 2022) with 3 numbers of c=c, polyunsaturated acid was modeled under unsaturated fat category. The coconut oil was selected as an example to model for the experimental purpose under the saturated fat/oil type due to it is the most usable and main edible (Seneviratne & Jayathilaka, 2016) saturated fat type in Sri Lanka. An edible vegetable oil type which is Canola oil (Dupain et al., 2007) is selected under the unsaturated fat type for modeling for further experiments due to higher utilization in the world (Statista, 2018) and not only that it is a fat type including both monounsaturated and polyunsaturated fatty acids.

Saturated Fat

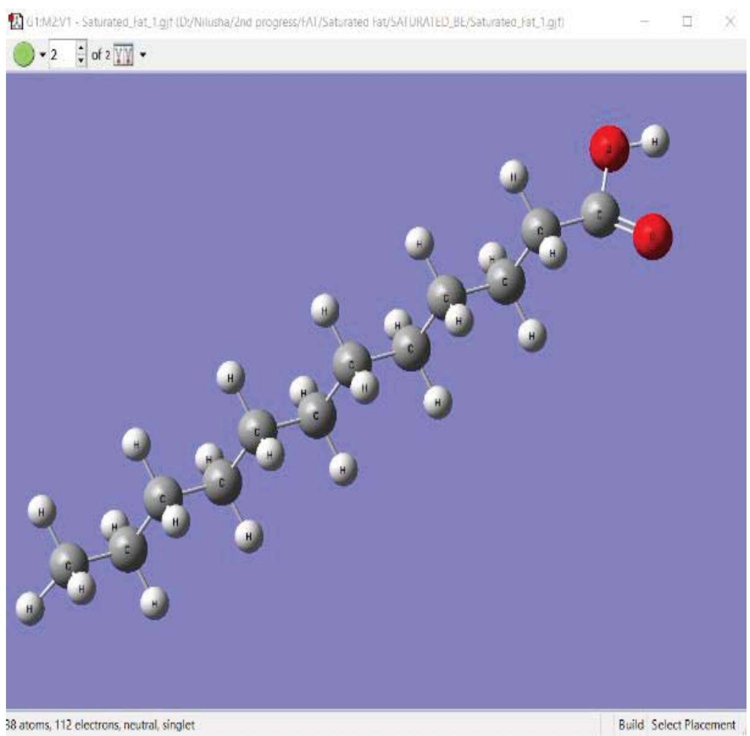


Figure 4.41: Modeled Saturated Fat Using GS

Unsaturated Fat

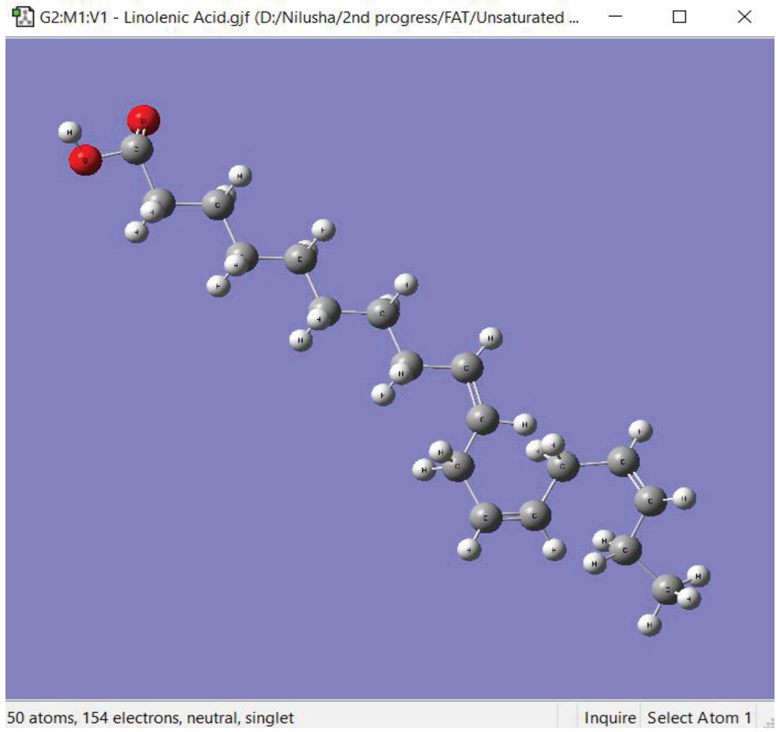


Figure 4.42: Modeled Unsaturated Fat Using GS

Coconut Oil

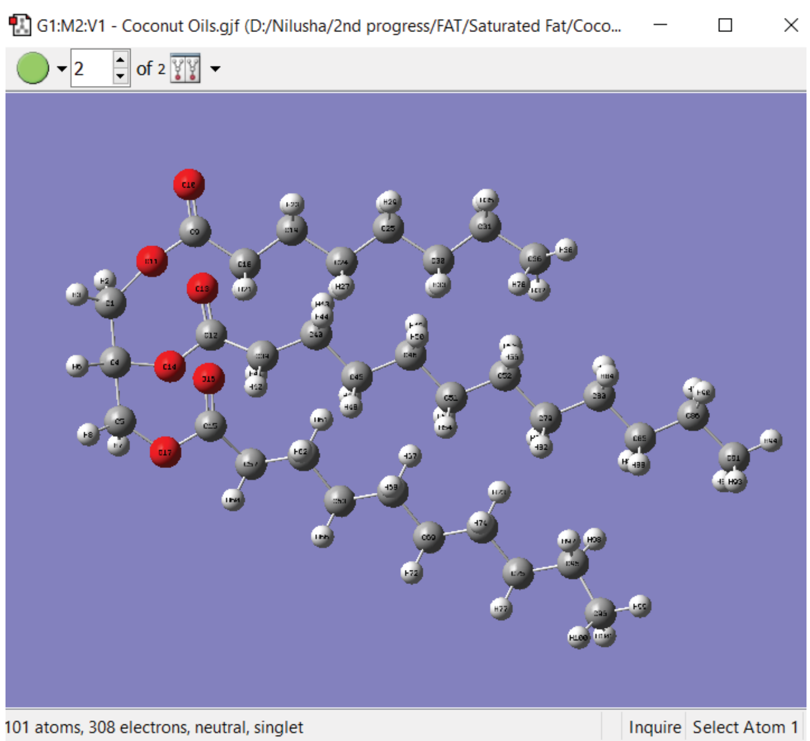


Figure 4.43: Modeled Coconut Oil Using GS

Vegetable Oil (Canola Oil)

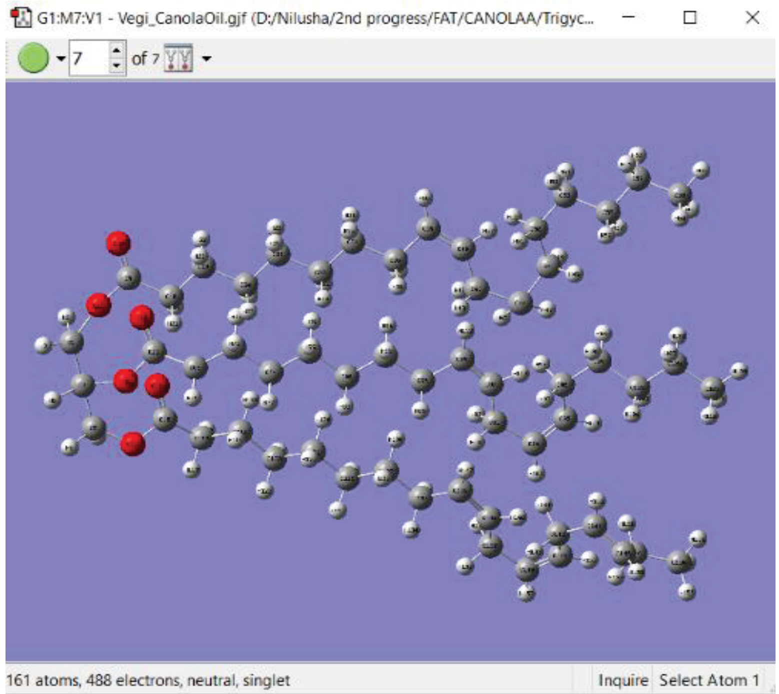


Figure 4.44: Modeled Vegetable Oil (Canola) Using GS

4.3.4.2 Calculated BEs of Red Clay and Fat/Oil (Saturated Fat, Unsaturated Fat, Coconut Oil and Vegetable Oil) Combinations

This section shows the individually calculated energy results of each saturated, unsaturated, coconut oil and vegetable oil (Canola oil) through the relevant figures of Gaussian Calculation Summery. At the same time system energies of relevant combinations after they couple with Red clay are shown through the relevant figures of Gaussian Calculation Summery. The sample screen shots of Gaussian Calculation Summery generated through GS are shown for Saturated fat individually and Red Clay and Saturated fat combinations and the same procedure was followed to other combinations including unsaturated fat, coconut oil and vegetable oil. The energy value for the Red clay was used as identified in Step 03. The calculated results for BEs of relevant combinations which are Red clay and saturated fat/oil, Red clay and unsaturated fat/oil, Red clay and coconut oil and then Red clay and vegetable oil are shown in the relevant tables below each figures accordingly. As previous calculation the au unit of relevant BEs was converted to kcal/mol.

These BE values are used to compare with the BEs which were obtained by combining each fat/oil type with the identified Apatite (mineral) + Red clay combination in Step 03.

Red Clay and Saturated Fat

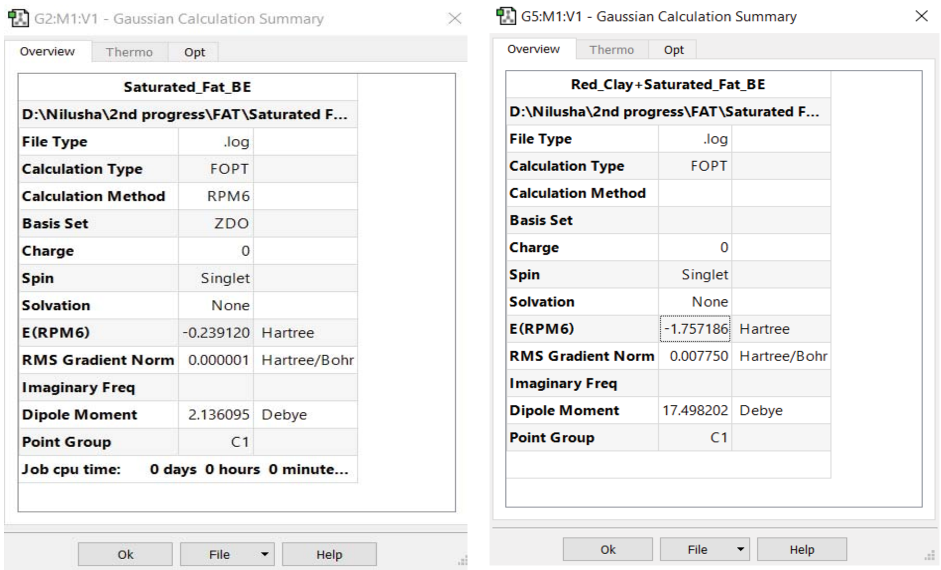


Figure 4.45: Gaussian Calculation Summery for Saturated Fat and for Red Clay and Saturated Fat System

Table 4.32: BE Calculation for Red Clay and Saturated Fat Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay + Saturated Fat		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Saturated Fat	-0.23912	
Mixture	-1.757186	
Binding Energy	-2.473995	-1552.431863

Red Clay and Unsaturated Fat

Table 4.33: BE Calculation for Red Clay and Unsaturated Fat Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay and + Unsaturated Fat (Linolenic)		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Unsaturated Fat	-0.17085	
Mixture	-2.62842	
Binding Energy	-3.413499	-2141.970623

Red Clay and Coconut Oil

Table 4.34: BE Calculation for Red Clay and Coconut Oil Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Coconut Oil		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Coconut Oil	-0.626464	
Mixture	-3.043719	
Binding Energy	-3.373184	-2116.67296

Red Clay and Vegetable Oil (Canola Oil)

Table 4.35: BE Calculation for Red Clay and Vegetable Oil (Canola Oil) Combination

$E_{(bind\ (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay and +Vegetable Oil (Canola Oil)		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay	0.955929	
Canola Oil	-0.586769	
Mixture	-2.055558	
Binding Energy	-2.424718	-1521.510545

4.3.4.3 Calculated BEs of Red Clay + Apatite Mixture with Fat/Oil Combinations

Red Clay+ Apatite and Saturated Fat

In this section the saturated, unsaturated, coconut oil and the vegetable oil were combined with Red clay and Apatite mixture which was identified in Step 03 as individual systems. The combinations are Red clay + Apatite and saturated fat, Red clay + Apatite and unsaturated fat, Red clay + Apatite and coconut and then Red clay + Apatite and vegetable oil. The Apatite and + Red clay was considered as a one compound and the relevant fat/oil type was the combined material to the mixture. Then the total energy values for each system were displayed in relevant figures of Gaussian Calculation Summery and the relevant BE values were calculated according to the formula were shown in relevant tables below accordingly. The sample screen shots of Gaussian Calculation Summery generated through GS are shown for Red clay + Apatite and saturated fat combinations in Figure 4.46 and the same procedure was followed to other combinations including unsaturated fat. Coconut oil and vegetable oil. The energy value for the Red clay + Apatite mixture was used which was calculated in Step 03.

Red Clay+ Apatite and Saturated Fat

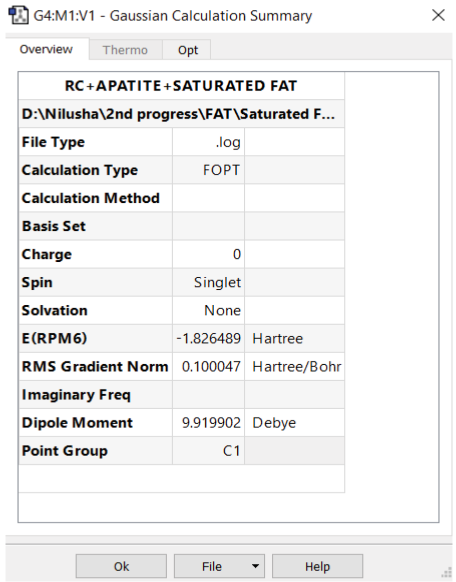


Figure 4.46: Gaussian Calculation Summery for Red Clay+ Apatite and Saturated Fat System

Table 4.36: BE Calculation for Red Clay+ Apatite and Saturated Fat Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay & Apatite + Saturated Fat		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay & Apatite	-6.705931	
Saturated Fat	-0.23912	
Mixture	-1.826489	
Binding Energy	5.118562	3211.897655

Red Clay+ Apatite and Unsaturated Fat

Table 4.37: BE Calculation for Red Clay+ Apatite and Unsaturated Fat Combination

$E_{(bind\ (mon1\text{-}mon2))} = E_{(opt\text{-}dimer)} - (E_{(opt\text{-}mon1)} + E_{(opt\text{-}mon2)})$		
Red Clay and Apatite + Unsaturated Fat (Linolenic)		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay + Apatite	-6.705931	
Unsaturated Fat	-0.17085	
Mixture	-3.090925	
Binding Energy	3.785856	2375.62464

Red Clay+ Apatite and Coconut Oil

Table 4.38: BE Calculation for Red Clay + Apatite and Coconut Oil Combination

$E_{(bind (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Apatite and Coconut Oil		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay + Apatite	-6.705931	
Coconut Oil	-0.626464	
Mixture	-3.428636	
Binding Energy	3.903759	2449.608773

Red Clay+ Apatite and Vegetable Oil (Canola Oil)

Table 4.39: BE Calculation for Red Clay + Apatite and Vegetable Oil (Canola Oil) Combination

$E_{(bind (mon1-mon2))} = E_{(opt-dimer)} - (E_{(opt-mon1)} + E_{(opt-mon2)})$		
Red Clay + Apatite and Vegetable Oil		
System	Electronic E (au)	Electronic E (kcal/mol)
Red Clay + Apatite	-6.705931	
Canola Oil	-0.586769	
Mixture	-1.072456	
Binding Energy	6.220244	3903.20311

4.3.4.4 Nonstick Property Performances through Binding Energy Analysis

The BE values calculated by using the formula was mentioned in the Table 4.40 and 4.41 for the comparison. Each BE between Red clay and fat/oil are shown in 2nd column and the BE values between Red clay + Apatite and fat/oil types are mentioned in 3rd column in Table 4.40. The same recording method was used for the example fat/oil types which are coconut and vegetable oil in Table 4.41. Two separate tables were displayed for general structures of saturated and unsaturated fat/oil types and for actually existing examples for saturated and unsaturated fat/oil types subsequently coconut oil and for vegetable oil. The final BE values in kcal/mol were rounded to the nearest whole number for easy reference.

Table 4.40: BE value comparison between Red clay+ fat/oil and Red Clay+ Apatite and fat/oil

Fat Type	BE (Red Clay + Fat)	BE (Red Clay + Apatite and Fat)
Saturated Fat	-1552	3212
Unsaturated Fat	-2142	2376

The BE for Red clay and saturated fat is-1552 kcal/mol and the BE value for Red clay and unsaturated fat is -2142 kcal/mol. The BE for Red Clay + Apatite and saturated fat is 3212 kcal/mol and the BE value for Red Clay + Apatite and unsaturated fat is

2376 kcal/mol. Therefore, the BE values of Red clay and fat/oil combinations are negative BE values and the BE values of Red Clay + Apatite, and fat/oil combinations are positive BE values. As per the BE value results the Figure 4.47 demonstrates the negative and positive BE value levels.

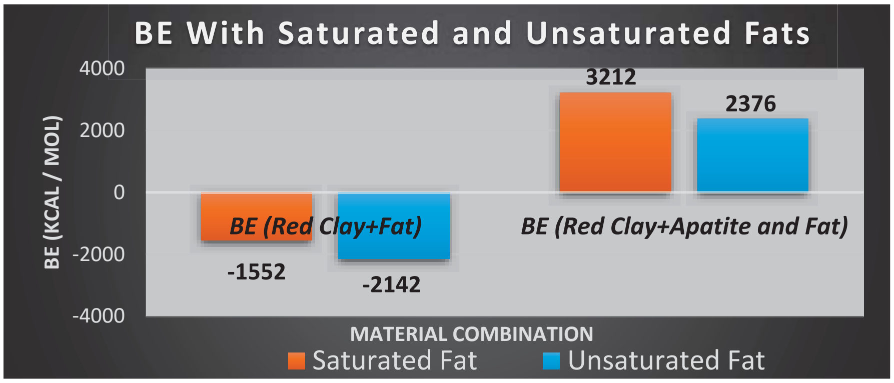


Figure 4.47: Negative and Positive BE value levels of Red clay+ fat/oil and Red Clay+ Apatite and fat/oil

The BE for Red clay and coconut oil is -2117 kcal/mol and the BE value for Red clay and Vegetable oil (Canola oil) is -1522 kcal/mol. The BE for Red Clay + Apatite and coconut oil is 2450 kcal/mol and the BE value for Red Clay + Apatite and vegetable oil (Canola oil) is 3903 kcal/mol. Thus, the BE values of Red clay and coconut oil/vegetable oil combinations are negative BE values and the BE values of Red Clay + Apatite, and coconut oil/vegetable oil combinations are positive BE values. As per the BE value results Figure 4.48 demonstrates the negative and positive BE value levels for relevant mixtures including coconut oil and vegetable oil.

Table 4.41: BE value comparison between Red clay + coconut oil/vegetable oil and Red Clay + Apatite and coconut oil/vegetable oil

Dietary Oil	BE (Red Clay + Dietary Oil)	BE (Red Clay+ Apatite and Dietary Oil)
Coconut Oil	-2117	2450
Vegetable Oil	-1522	3903

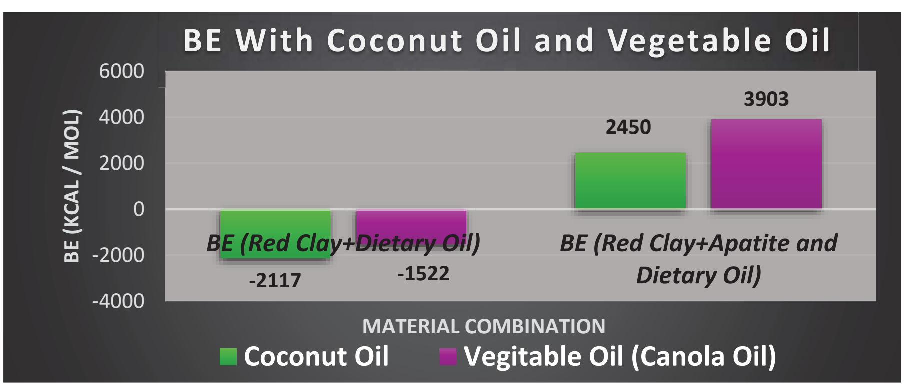


Figure 4.48: Negative and Positive BE value levels of Red clay+ coconut oil/vegetable oil and Red Clay+ Apatite and coconut oil/vegetable oil

According to these results more stable systems are generated between Red clay and saturated /unsaturated combinations than Red Clay+ Apatite and fat/oil combinations due to their negative BEs. As mentioned in literature review the exothermic reactions have occurred during when energy values are negative. Hence the intermolecular interaction energy between Red clay and fat/oil are higher than the same mixture with the Apatite mineral.

According to the results, stability is not changed whether it is saturated fat, unsaturated fat, coconut or vegetable oil because they have negative BEs only with the Red clay combination. Even though, the Red clay mixture with Apatite mineral generate unstable intermolecular interactions with saturated fat, unsaturated fat, coconut or vegetable oil because they show positive BE values.

Figure 4.49: Stickiness of Red Clay +Fat/Oil and Red Clay + Apatite and Fat/Oil

Thus, as per Figure 4.49 the stickiness of fat/oil to the Red clay is higher than the same Red clay mixture including Apatite mineral. The Red clay + Apatite mixture has the low nonstick ability to the fat/oil. Therefore, using Apatite mineral with Red clay is caused to increase the nonstick property of the pottery making material.

4.4 Summary

This chapter presents the results and in-depth discussions derived from industry survey, a comprehensive literature review on identified industrial clay and minerals in Sri Lanka, and computational analyses including modeling clay and mineral molecules and binding energy calculations using GS under computational chemistry. These findings pertain to identify the best collaborative mineral material to clay to make cooking clay potteries and analyze the nonstick property of recognized clay and mineral combination in the context of the overarching research aims and objectives.

Although Red clay, Ball clay, and White clay are identified as the primary industrial clay types available in Sri Lanka according to the literature, based on industrial investigations approximately 90% of pottery manufacturers utilize Red clay specifically for the production of cooking pottery. Sri Lanka is rich in a variety of industrial non-metallic minerals, with significant occurrences of Kaolin, Montmorillonite, Graphite, Ilmenite, Rutile, Zircon, Quartz, Feldspar, Clay, Apatite, Silica Sand, Garnet Sand, Mica, Calcite, and Dolomite.

In the pottery manufacturing sector, three distinct types of production centers were identified, which are medium-scale enterprises, small-scale domestic manufacturing units, and government sponsored clay-based craft villages and training centers. Analysis of Red clay utilization across these categories indicates that small-scale domestic manufacturing units exhibit the highest usage of Red clay. Furthermore, this category represents the predominant form of industrial activity within the investigated pottery production centers.

Gender participation analysis within the clay pottery industry reveals that male involvement is predominant compared to the other two categories which are female only and both male and female participation. Notably, both males and females are largely engaged in small-scale domestic pottery production. In contrast, male participation spans all three industry types that are medium-scale enterprises, small-scale domestic manufacturing centers, and government-sponsored clay-based craft villages and training centers.

Investigations exhibit that, in addition to culinary clay pottery, a range of other clay-based products are manufactured, including seasonal items such as milk pottery. In contrast, cooking clay pottery is produced consistently throughout the year, indicating its sustained demand and central role in the industry.

The general cooking clay pottery production process consists of collecting the secondary clay (earthenware clay), making the clay mix by adding water and sand, cleaning the clay mix and blend it again, cleaning the clay mix and blend it again with water, sand and silicon to get the correct seasoning level, keeping the clay mix for season nearly 1-2 days, making cookware using “sakaporuwa” or mould , letting it to dry under shade, loading in the oven to burn and lastly unloading the pots from the oven to let it to cool.

Based on the binding energy calculations on modeled clay and minerals by using GS between Red clay and selected mineral additives, the Red clay + Apatite system exhibits the highest binding energy value of –3177 kcal/mol among other combinations. This indicates that the Red clay + Apatite combination forms the most stable system among the evaluated mineral combinations, characterized by strong intermolecular interactions and enhanced structural compatibility.

The non-stick performance of the Red clay + Apatite mixture was assessed through BE calculations with various saturated fat, unsaturated fat, coconut oil and vegetable oil. The BEs for Red clay in combination with saturated fat, unsaturated fat, coconut oil, and vegetable oil were found to be negative, with values of –1552, –2142, –2117, and –1522 kcal/mol, respectively. These negative values indicate strong intermolecular interactions and stable systems. In contrast, the binding energies for the Red clay + Apatite mixture with the same fat/oil types were all positive values which were 3212, 2376, 2450, and 3903 kcal/mol that suggesting weaker and less stable interactions to the saturated fat, unsaturated fat, coconut oil and vegetable oil. This comparative analysis implies that pure Red clay exhibits stronger affinity toward fats and oils than the Red clay + Apatite mixture. Thereby a superior non-stick property was shown in the Red clay + Apatite mixture compared to the individual Red clay.

CHAPTER 5

CONCLUSION, RECOMMONDATIONS AND FUTURE WORK

5.1 Conclusions

The first objective of this study was to identify the industrial need of developing proper nano material to use in clay pottery which is used for cuisine purposes. The comprehensive literature review was conducted to identify the industrial need with parallel to research gap identification. There are two main problems that have been identified which are caused to generate industrial needs and they are using metal and nonstick metal cookware cause hygienic problems in human beings and food stickiness to the inner surface of the clay pottery during cooking.

The second objective was to identify the proper material which can be used as nanomaterial for clay pottery. Previous studies show, using metal and metal nonstick cookware are caused to hygienic problems in humans and people tend to avoid using them and find alternative cooking pottery which is not harmful for human health. Nevertheless, with the current busy schedule there should be advancements as well as the non-harmful to human health. Hence the property advancement of clay pottery making material focusing on the nonstick property improvement, was done with a natural nonmetallic mineral in Sri Lanka by using computational chemistry.

Under this step, the primary data collected through the industrial survey revealed that Red clay is the most usable clay type which is used for cooking clay pottery. As Sri Lanka is a natural clay and mineral rich country and due to the favorable properties of clay to the human consumption, it was experimented to develop the cooking clay pottery material by collaborating a suitable clay and mineral material. The literature review illustrates the Red clay, Ball clay, and White clay are the most usable clay types in clay industry in Sri Lanka. At the same time Kaolin, Montmorillonite, Graphite, Ilmenite, Rutile, Zircon, Quartz, Feldspar, Kaolin, Apatite, Silica Sand, Garnet sand, Mica, Calcite and Dolomite have been recognized as the abundant industrial nonmetallic minerals in Sri Lanka. The relevant chemical and physical properties of these clay and minerals which were extracted through the literature review, particularly the chemical formula and structures were used to design them to simulate. The GS under computational chemistry was used to simulate and find out the relevant BEs to decide the most suitable clay and mineral combination. Considering the Binding Energies between identified Red clay and selected minerals, the Red clay and Apatite combination shows the highest negative Binding Energy -3177 kcal/mol compared to other mineral combinations. Hence, Red clay and Apatite combination is the most stable system with strong intermolecular interaction among other combinations. Thus, Red Clay and Apatite combination is the most suitable blend for developing a material for nonstick clay pottery.

The final objective was to analyze the performances of the identified clay and mineral combination for nano composite. The fat/oil as a staple food type in human type, it was used to analyze the nonstick property of the clay + mineral combination. The nonstick property performances of the identified Red clay and Apatite mixture were experimented through the BEs by combining this mixture with fat/oil. When considering BEs of the combinations of Red clay with each saturated fat, unsaturated fat, coconut oil and vegetable oil are negative values which are -1552, -2142, -2117 and -1522 kcal/mol. When considering BEs of the combinations of Red clay + Apatite mixture with each saturated fat, unsaturated fat, coconut oil and vegetable oil are positive values which are 3212, 2376, 2450 and 3903 kcal/mol.

Therefore, the most stable combinations are shown between only the Red clay and relevant fat/oil. However, the combined systems were unstable when with the Apatite in the Red clay mixture. Therefore, there are less strong intermolecular interactions between the Red clay + Apatite mixture and fat/oil.

Moreover, the industrial survey demonstrates there are three types of pottery making centers which are medium-scale, small-scale domestic manufacturing centers and government sponsored clay-based creations village and training centers among the investigated clay centers. In analysis of Red clay usage among these industry types, the small-scale domestic manufacturing centers have the highest usage, and majority of the industrial type is small-scale domestic manufacturing center type. In analyzing the gender participation with clay pottery industry, the male contribution is higher than other two types and they are female and both male and female involvement in the industry. Mostly both females and males are involving in small scale domestic type pottery making industry. Meanwhile the males are involving in all medium-scale, small-scale domestic manufacturing centers and government sponsored clay-based creations village and training center industries. According to investigations there are other clayware in addition to cooking clay potteries and others are some seasonal products like milk pots and cooking clay potteries are made throughout the whole year.

In conclusion, this research has created a significant implementation in developing a proper nanomaterial to use in cooking clay pottery. It shows that the metal and nonstick metal cooking vessels badly affect human health and the food stickiness to the clay pottery are the problems faced during the cooking. With creating improved cooking clay pottery, Red clay has identified most usable clay type which is used for making cooking clay pottery in Sri Lanka and the collaborating with Apatite mineral is shown the increased nonstick property of Red clay and Apatite compound. This combination avoids the sticking of edible fat/oil to the surface. Thus, the use of Apatite mineral with Red clay, enhances the nonstick property of clay and mineral composite of the clay pottery making material by avoiding food stickiness to the pottery material during cooking.

The applying of nano technology increases the BE when the particle size reduces. Therefore, the nano size particles lead to high binding energy, and it causes them to generate more steady system when using nano size particles for Red clay and Apatite mixture for pottery making compound.

5.2 Recommendations

Based on the findings and conclusions the following recommendations can be shown.

- The metal and nonstick metal cooking vessels badly affect human health, and the alternative property improved nonstick clay cookware can be produced by collaborating Red clay with Apatite mineral.
- Even though the Red clay, Ball clay and White clay are the mainly existing industrial clay types in Sri Lanka, Red clay is considered as the most suitable and widely used clay type for manufacturing cooking pottery in Sri Lanka from the past. When utilizing Red clay for cooking pottery, both the consistency of raw material supply and the purity of the Red clay must be carefully managed to ensure the quality and performance of the final pottery products.
- According to the calculated BEs through the GS the Red clay and Apatite mixture is the most appropriate combination to make pottery making material and Apatite mineral's supply and the purity should be considered during making the Red clay and Apatite mixture. The making of materials as suitable for the collaboration to make the cooking pottery material should be done in a proper way focusing on increasing the nonstick property of the overall mixture. Application of nano technology in making nano particles of Red clay and Apatite mixture will enhance the properties including nonstick property of the developed pottery material and the nanoparticle making should be done through an appropriate process.
- According to the industrial survey, not only that the medium scale clay pottery making centers also are maintained at a considerable level and Sri Lankan government also provides the facilitates to maintain government sponsored clay-based creations village and training centers. However, there is a deficiency of large-scale clay pottery making centers in investigated areas and potential is with establishing large scale pottery centers with increasing the involving of new technology for clay pottery industry.
- The individual female contribution in pottery making industry is very low. Therefore, the involvement of both male and female contribution in clay industry should be increased at least in medium scale type to develop the clay industry in Sri Lanka. Nonetheless there is a possibility to increase both male and female contribution in pottery industry through continuous awareness conduct by the clay base centers which are established by the government.

Therefore, the cooking clay pottery industry holds significant potential for value-added product development by enhancing functional properties, particularly nonstick performance through the incorporation of Apatite, a compatible mineral additive, into the widely utilized Red clay. This approach offers a sustainable alternative to conventional metal and synthetic nonstick cookware, which are associated with potential health risks.

5.3 Future Work

- The identification of the Apatite as the most suitable mineral additive and the evaluation of the nonstick properties of the Red clay and Apatite composite were conducted through computational chemistry simulations using Gaussian software. As these results are based solely on theoretical modeling, experimental validation under controlled laboratory conditions is essential. This includes synthesizing the actual Red clay and Apatite composite and assessing its performance in enhancing the nonstick properties of clay cookware.
- The nanoscale synthesis of the Red clay and Apatite composite represents a critical aspect of this research, as it will be expected to significant enhancement of the nonstick properties compared to the use of conventionally prepared Red clay and Apatite materials.

REFERENCES

Abdelrasoul, A., Zhang, H., Cheng, C.-H., & Doan, H. (2017). Applications of molecular simulations for separation and adsorption in zeolites. *Microporous and Mesoporous Materials*, *242*, 294–348. https://doi.org/10.1016/j.micromeso.2017.01.038

Abdulla, N. (2024, September). UAE residents warned of "teflon flu"; high-temperature nonstick pans linked to fever [Review of *UAE residents warned of "teflon flu"; high-temperature nonstick pans linked to fever*]. *Health*. https://www.khaleejtimes.com/lifestyle/health/uae-residents-warned-of-teflon-flu-high-temperature-nonstick-pans-linked-to-fever

Abid, N., Khan, A. M., Shujait, S., Chaudhary, K., Ikram, M., Imran, M., Haider, J., Khan, M., Khan, Q., & Maqbool, M. (2022). Synthesis of nanomaterials using various top-down and bottom-up approaches, influencing factors, advantages, and disadvantages: A review. *Advances in Colloid and Interface Science*, *300*, 102597. https://doi.org/10.1016/j.cis.2021.102597

Adhikari, J., & Adhikari, R. (2023). Free and Open Source Codes for Computational Chemistry Research Initiation: A Conspectus. *Journal of Nepal Chemical Society*, *43*(2), 11–22. https://doi.org/10.3126/jncs.v43i2.53337

Admin. (2024, March 4). *Unlocking the Molecular Universe: Essential Tools and Software in Computational Chemistry - IM Group Of Researchers - An International Research Organization*. IM Group of Researchers - an International Research Organization. https://imgroupofresearchers.com/unlocking-the-molecular-universe-essential-tools-and-software-in-computational-chemistry/

Adminecoveya. (2025, March 21). *How to Care for Clay Cookware: Tips for Long-Lasting Use*. Ecoveya. https://ecoveya.com/how-to-take-care-of-your-clay-cookware-for-long-lasting-use/

Akay, M. B., Şener, K., Sari, S., & Bodur, E. (2022). Inhibitory Action of Omega-3 and Omega-6 Fatty Acids Alpha-Linolenic, Arachidonic and Linoleic acid on Human Erythrocyte Acetylcholinesterase. *The Protein Journal*. https://doi.org/10.1007/s10930-022-10088-z

Al Ani, T., & Sarapää, O. (2008). CLAY AND CLAY MINERALOGY PHYSICAL – CHEMICAL PROPERTIES AND INDUSTRIAL USES [Review of *CLAY AND CLAY MINERALOGY PHYSICAL – CHEMICAL PROPERTIES AND INDUSTRIAL USES*]. In *Geological Survey of Finland* (pp. 11–65). Geological Survey of Finland. https://www.researchgate.net/publication/292706105

Alabi, O. A., & Adeoluwa, Y. M. (2020). Production, Usage and Potential Public Health Effects of Aluminum Cookware: A Review. *Annals of Science and Technology*, *5*(1), 20–30. https://doi.org/10.2478/ast-2020-0003

Amar, I.,Hami, B., Chouaib, A.C., & Boudjema, B.B. (2012). Rheological Behavior of the Epoxy Resin Loaded with the Pozzolan. *Materials Science and Engineering A* 2(7), 519-524. DOI: 10.17265/2161-6213/2012.07.005

Amboro, J. L., Purwasito, A., & Warto, N. (2022). The characteristics of teapots made of plastic and clay: what are their designs, functions, and impacts on the environment? *IOP Conference Series: Earth and Environmental Science*, *1114*(1), 012110–012110. https://doi.org/10.1088/1755-1315/1114/1/012110

Asbury Carbons. (2025). *Graphite Structure*. Asbury.com. https://www.asbury.com/resources/education/graphite-101/structural-description/

ASDN. (2025). *Silicates.* Asdn.net. https://asdn.net/asdn/chemistry/silicates.php

Asia InCH. (2017). *Earthenware of Sri Lanka* [Review of *Earthenware of Sri Lanka*]. Https://Asiainch.org; The Craft Revival Trust. https://asiainch.org/craft/earthenware/#photos_section

Awasthi, A., Jadhao, P., & Kumari, K. (2019). Clay nano-adsorbent: structures, applications and mechanism for water treatment. *SN Applied Sciences*, *1*(9). https://doi.org/10.1007/s42452-019-0858-9

Azevedo, D. H. M., Fabris, G. S. L., Sambrano, J. R., & Cordeiro, J. M. M. (2020). Surface and electronic properties of rutile TiO2 thin films coated with PbO2. *Computational Materials Science*, *171*, 109222. https://doi.org/10.1016/j.commatsci.2019.109222

Bansal, C., & Zaina, S., & Parihar, V. (2020). REVIEW ON HEALTH IMPACT OF HAZARDOUS AND SAFEST TRADITIONAL COOKWARE WITH AYURVEDIC APPROACH. *AYUSHDHARA*, *7*(1), 2559-2566. https://doi.org/10.47070/ayushdhara.v7i1.519

Bantie, Z., Tezera, A., Abera, D., & Nega, T. (2024). Nanoclays as fillers for performance enhancement in building and construction industries: State of the art and future trends. *IntechOpen EBooks*. https://doi.org/10.5772/intechopen.1005147

Beckford, S., Cai, J., Fleming, R. A., & Zou, M. (2016). The Effects of Graphite Filler on the Tribological Properties of Polydopamine/PTFE Coatings. *Tribology Letters*, *64*(3). https://doi.org/10.1007/s11249-016-0777-5

Bloomfield, L. (2016). clay structure [Review of *clay structure*]. In www.ceramicsmonthly.org . Techno File.

Burnham, A. D. (2018). Zircon. *Reference Module in Earth Systems and Environmental Sciences*. https://doi.org/10.1016/b978-0-12-409548-9.10911-x

Caroline, A., Oliveira, J., Jury, V., Boillereaux, L., & João Borges Laurindo. (2021). Adhesion of Food on Surfaces: Theory, Measurements, and Main Trends to Reduce It Prior to Industrial Drying. *Food Engineering Reviews (Print)*, *13*(4), 884–901. https://doi.org/10.1007/s12393-021-09286-9

ChemicalBook. (2017). *14808-60-7(Quartz) Product Description.* *https://www.chemicalbook.com/ChemicalProductProperty_US_CB9154858.aspx*

ChemicalBook. (2023). *Ilmenite (FeTiO3).* *https://www.chemicalbook.com/ProductChemicalPropertiesCB1904228_EN.htm*

Christensen, A. S., Kubař, T., Cui, Q., & Elstner, M. (2016). Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. *Chemical Reviews*, *116*(9), 5301–5337. https://doi.org/10.1021/acs.chemrev.5b00584

Coxworth, B. (2018, December 13). *Fat-trapping clay may form part of a treatment for obesity*. New Atlas. https://newatlas.com/clay-fat-obesity/57661/

Coyle, D. (2023, May 19). *Is Nonstick Cookware Like Teflon Safe to Use?* Healthline; Healthline Media. https://www.healthline.com/nutrition/nonstick-cookware-safety

Desk, T. L. (2024, July 24). *Teflon flu is rising in US; symptoms, dos and don’ts while cooking in non-stick cookware*. The Times of India; Times Of India. https://timesofindia.indiatimes.com/life-style/health-fitness/health-news/teflon-flu-is-rising-in-us-symptoms-dos-and-donts-while-cooking-in-non-stick-cookware/articleshow/111973109.cms

Dhiman, N. K., Sidhu, N., Agnihotri, S., Mukherjee, A., & Reddy, M. V. (2022). *Role of nanomaterials in protecting building materials from degradation and deterioration*. 405–475. https://doi.org/10.1016/b978-0-12-823970-4.00024-5

Dhote, V. K., Dhote, K., Pandey, S. P., Shukla, T., Maheshwari, R., Mishra, D. K., & Tekade, R. K. (2019). Fundamentals of Polymers Science Applied in Pharmaceutical Product Development. *Elsevier EBooks*, 85–112. https://doi.org/10.1016/b978-0-12-817909-3.00003-0

Dopfer, D., Palzer, S., Heinrich, S., Fries, L., Antonyuk, S., Haider, C., & Salman, A. D. (2013). Adhesion mechanisms between water soluble particles. *Powder Technology*, *238*, 35–49. https://doi.org/10.1016/j.powtec.2012.06.029

Du, Z., & Zhu, X. (2019). Molecular Dynamics Simulation to Investigate the Adhesion and Diffusion of Asphalt Binder on Aggregate Surfaces. *Transportation Research Record: Journal of the Transportation Research Board*, *2673*(4), 500–512. https://doi.org/10.1177/0361198119837223

Dupain, X., Costa, D. J., Schaverien, C. J., Makkee, M., & Moulijn, J. A. (2007). Cracking of a rapeseed vegetable oil under realistic FCC conditions. *Applied Catalysis B: Environmental*, *72*(1-2), 44–61. https://doi.org/10.1016/j.apcatb.2006.10.005

Export Development Board Sri Lanka (2020). *Mineral Resources Found in Sri Lanka*. https://www.srilankabusiness.com/blog/clay-industry-sri-lanka.html

Export Development Board Sri Lanka (2021). *Mineral Resources Found in Sri Lanka*. https://www.srilankabusiness.com/blog/mineral-resources-from-sri-lanka.html

Febrida, R., Setianto, S., Herda, E., Cahyanto, A., & Joni, I. M. (2021). Structure and phase analysis of calcium carbonate powder prepared by a simple solution method. *Heliyon*, *7*(11), e08344. https://doi.org/10.1016/j.heliyon.2021.e08344

Gaussian.com. (2019). *Gaussian.com | Expanding the limits of computational chemistry*. https://gaussian.com/

Geiger, S. D., Xiao, J., Ducatman, A., Frisbee, S., Innes, K., & Shankar, A. (2014). The association between PFOA, PFOS and serum lipid levels in adolescents. *Chemosphere*, *98*, 78–83. https://doi.org/10.1016/j.chemosphere.2013.10.005

Geology Science. (2018, April 17). *Zircon Mineral | Physical - Optical Properties, Occurrence, Uses*. Geology Science. https://geologyscience.com/minerals/zircon/

Gerardu, T., Dijkstra, J., Beeltje, H., van Renesse van Duivenbode, A., & Griffioen, J. (2023). Accumulation and transport of atmospherically deposited PFOA and PFOS in undisturbed soils downwind from a fluoropolymers factory. *Environmental Advances*, *11*, 100332. https://doi.org/10.1016/j.envadv.2022.100332

Ginneken, V. V., Elwin Verheij, & Van, J. (2019). IMPACT OF THE “WRONG” FATS ON THE COMPOSITION OF THE HEART MUSCLE IN AN OBESE HIGH FAT DIET INDUCED INSULIN RESISTANT C57BL6 MOUSE MODEL FOLLOWING A LIPIDOMICS SYSTEMS BIOLOGY LCMS

APPROACH. *European Journal Pharmaceutical and Medical Research, 6(2),* 243–262. https://www.researchgate.net/publication/330811700

Good, A. C., Hodgkin, E. E., & Richards, W. G. (1992). Utilization of Gaussian functions for the rapid evaluation of molecular similarity. *Journal of Chemical Information and Computer Sciences*, *32*(3), 188–191. https://doi.org/10.1021/ci00007a002

Greathouse, J. A., & Cygan, R. T. (2013). *Molecular Simulation of Clay Minerals*. 405–423. https://doi.org/10.1016/b978-0-08-098259-5.00016-0

Greenberg, M. I., & Vearrier, D. (2015). Metal fume fever and polymer fume fever. *Clinical Toxicology*, *53*(4), 195–203. https://doi.org/10.3109/15563650.2015.1013548

Grew, E. S., Locock, A. J., Mills, S. J., Galuskina, I. O., Galuskin, E. V., & Halenius, U. (2013). Nomenclature of the garnet supergroup. *American Mineralogist*, *98*(4), 785–811. https://doi.org/10.2138/am.2013.4201

Harvard T.H. Chan School of Public Health. (2014). *Types of Fat*. The Nutrition Source. https://nutritionsource.hsph.harvard.edu/what-should-you-eat/fats-and-cholesterol/types-of-fat/

Hashemi, N., Milani, E., Mortezavi, S. A., & Yazdi, F. T. (2017). Sticky point temperature as a suitable method in evaluation of shelf life of food powders. *Bulletin de La Société Royale Des Sciences de Liège*, *86,* 7–12. https://doi.org/10.25518/0037-9565.6519

Hatzikiriakos, S. G. (2012). Rheology and Processing of Tetrafluoroethylene/Hexafluoropropylene Copolymers. *International Polymer Processing*, *27*(2), 167–180. https://doi.org/10.3139/217.2539

Hazrah, K. S., & Antao, S. M. (2022). Apatite, Ca10(PO4)6(OH,F,Cl)2: Structural Variations, Natural Solid Solutions, Intergrowths, and Zoning. *Minerals*, *12*(5), 527. https://doi.org/10.3390/min12050527

Hehre, W. J. (2003). *A guide to molecular mechanics and quantum chemical calculations*. Wavefunction.

Holland, J. P., Ferdani, R., Anderson, C. J., & Lewis, J. S. (2009). Copper-64 Radiopharmaceuticals for Oncologic Imaging. *PET Clinics*, *4*(1), 49–67. https://doi.org/10.1016/j.cpet.2009.04.013

Hollingsworth, S. A., & Dror, R. O. (2018). Molecular Dynamics Simulation for All. *Neuron*, *99*(6), 1129–1143. https://doi.org/10.1016/j.neuron.2018.08.011

Isaifan, R. J., Ntais, S., & Baranova, E. A. (2013). Particle size effect on catalytic activity of carbon-supported Pt nanoparticles for complete ethylene oxidation. *Applied Catalysis A: General*, *464-465*, 87–94. https://doi.org/10.1016/j.apcata.2013.05.027

Ismaeili, J., & Patel, J., & Övez, B. (2022). Conceptual Study of Non-Stick Cookware Coatings and the Effect of Some Corresponding Additives on Their Performance. *Scientific Research Communications*, *2*(2), 1–15. https://doi.org/10.52460/src.2022.007

Jensen, F. (2017). *Introduction to Computational Chemistry* (Third Edition) [Review of *Introduction to Computational Chemistry*]. John Wiley & Sons, Ltd. http://dl.iranchembook.ir/ebook/Physical-Chemistry-723.pdf

Johansson, M. P., Kaila, V. R. I., & Sundholm, D. (2012). Ab Initio, Density Functional Theory, and Semi-Empirical Calculations. *Methods in Molecular Biology*, 3–27. https://doi.org/10.1007/978-1-62703-017-5_1

Karthik, K., Srilatha, P., Madhukesh, Khan, J. K., U., B.C. Prasannakumara, Kumar, R., Ishak, A., Hussain, S. M., Muhammad, T., & Abdou, M. (2024). Computational examination of heat and mass transfer of nanofluid flow across an inclined cylinder with endothermic/exothermic chemical reaction. *Case Studies in Thermal Engineering*, *57*, 104336–104336. https://doi.org/10.1016/j.csite.2024.104336

Kausar, A. (2020). *Flame retardant potential of clay nanoparticles* (pp. 169–184). Elsevier. https://doi.org/10.1016/B978-0-12-816783-0.00007-4

L'Annunziata, M. F. (2016). The Atomic Nucleus. *Elsevier EBooks*, 679–728. https://doi.org/10.1016/b978-0-444-63489-4.00020-4

Lee, C. H., Guo, Y. L., Tsai, P. J., Chang, H. Y., Chen, C. R., Chen, C. W., & Hsiue, T. R. (1997). Fatal acute pulmonary oedema after inhalation of fumes from polytetrafluoroethylene (PTFE). *European Respiratory Journal*, *10*(6), 1408–1411. https://doi.org/10.1183/09031936.97.10061408

Lee, J. Y., Lim, D. P., & Lim, D. S. (2007). Tribological behavior of PTFE nanocomposite films reinforced with carbon nanoparticles. *Composites Part B: Engineering*, *38*(7-8), 810–816. https://doi.org/10.1016/j.compositesb.2006.12.006

Lee, S. (2025). *Gaussian for Materials Science: A Practical Guide*. Numberanalytics.com. https://www.numberanalytics.com/blog/practical-gaussian-materials-science

Lehtola, S., & Karttunen, A. J. (2022). Free and open source software for computational chemistry education. *WIREs Computational Molecular Science*. https://doi.org/10.1002/wcms.1610

LookChem. (2008). *Dolomite (CaMg(CO3)2).* https://www.lookchem.com/Dolomite-CaMg-CO3-2-/

Malyshkina, M. V., & Novikov, A. S. (2021). Modern Software for Computer Modeling in Quantum Chemistry and Molecular Dynamics. *Compounds*, *1*(3), 134–144. https://doi.org/10.3390/compounds1030012

Mannar, M. G. V., & Wesley, A. S. (2017). *Food Fortification*. 143–152. https://doi.org/10.1016/b978-0-12-803678-5.00160-0

Marć, M., Kupka, T., Wieczorek, P. P., & Namieśnik, J. (2018). Computational modeling of molecularly imprinted polymers as a green approach to the development of novel analytical sorbents. *TrAC Trends in Analytical Chemistry*, *98*, 64–78. https://doi.org/10.1016/j.trac.2017.10.020

Marion, R., & Carrère, V. (2018). Mineral Mapping Using the Automatized Gaussian Model (AGM)—Application to Two Industrial French Sites at Gardanne and Thann. *Remote Sensing*, *10*(1), 146–146. https://doi.org/10.3390/rs10010146

MATMATCH. (2024). *Graphite: Properties, Occurrence and Applications. https://matmatch.com/learn/material/graphite*

Matyszczak, G., Jasiak, C., Rusinkiewicz, G., Domian, K., Brzozowski, M., & Krawczyk, K. (2025). Mathematical Modeling of Properties and Structures of Crystals: From Quantum Approach to Machine Learning. Crystals, 15(1), 61–61. https://doi.org/10.3390/cryst15010061

Michalski, M. C., Desobry, S., Pons, M. N., & Hardy, J. (1998). Adhesion of edible oils to food contact surfaces. *Journal of the American Oil Chemists' Society*, *75*(4), 447–454. https://doi.org/10.1007/s11746-998-0247-9

Mineralogy Database. (2014). *Apatite Mineral Data.* https://www.webmineral.com/data/Apatite.shtml

Mourik, T., Bühl, M., & Gaigeot, M.-P. (2014). Density functional theory across chemistry, physics and biology. *Philosophical Transactions. Series A, Mathematical, Physical, and Engineering Sciences*, *372*(2011). https://doi.org/10.1098/rsta.2012.0488

Muttashar, H. L., Hussin, M. W., Mohd Ariffin, M. A., Mirza, J., Hasanah, N., & Shettima, A. U. (2017). MECHANICAL PROPERTIES OF SELF-COMPACTING GEOPOLYMER CONCRETE CONTAINING SPENT

GARNET AS REPLACEMENT FOR FINE AGGREGATE. *Jurnal Teknologi*, *79*(3). https://doi.org/10.11113/jt.v79.9957

Nandadeva, B. D. (2017, September 8). *Pottery | The Encyclopedia of Crafts in WCC-Asia Pacific Region (EC-APR)*. Encyclocraftsapr.com. https://encyclocraftsapr.com/pottery-2/

Nano Research Element. (2025). *Montmorillonite bentonite clay* [Review of *Montmorillonite bentonite clay*]. https://www.nanorh.com/product/montmorillonite-bentonite-clay-al2o34sio2h2o-purity-99-9-8-10%C2%B5m/

Nanografi Advanced Materials. (2019). Nanoclay: Properties, Production, Applications [Review of *Nanoclay: Properties, Production, Applications*]. *Nanografi.com*. https://shop.nanografi.com/blog/nanoclay-properties-production-applications/

Nanografi Advanced Materials. (2024). How to Make Liquid Nanoclay? [Review of *How to Make Liquid Nanoclay?*]. *Nanografi.com*. https://shop.nanografi.com/blog/how-to-make-liquid-nanoclay/

National Institute of Standards and Technology. (2022). *What's a hartree?* [Review of *What's a hartree?*]. *Standard Reference Database 101*(22). Computational Chemistry Comparison and Benchmark DataBase. https://cccbdb.nist.gov/hartreex.asp

National Library of Medicine. . (2024). *compound Summary Kaolin***.** https://pubchem.ncbi.nlm.nih.gov/compound/Kaolin

Newbasics. (2021). Advantages and Disadvantages of using Clayware – Earthenware – Terracotta [Review of *Advantages and Disadvantages of using Clayware – Earthenware – Terracotta*]. *Clay Pots, Earthenware*. https://newbasics.in/2021/11/26/advantages-and-disadvantages-of-using-clayware-earthenware-terracotta/?srsltid=AfmBOooBEGaZ8kOyGzSBENH1KNDmLr3EIi7ApY-t7IN-PtxKmVfBw9qp

Nian, B., Xu, Y.-J., & Liu, Y. (2021). Molecular dynamics simulation for mechanism revelation of the safety and nutrition of lipids and derivatives in food: State of the art. *Food Research International*, *145*, 110399. https://doi.org/10.1016/j.foodres.2021.110399

Ntim, S. A., Norris, S., Scott, K., Thomas, T. A., & Noonan, G. O. (2018). Consumer use effects on nanoparticle release from commercially available ceramic cookware. *Food Control*, *87*, 31–39. https://doi.org/10.1016/j.foodcont.2017.12.003

Nurdin, R. (2024, August). Teflon Flu on the Rise: What Doctors Need to Know About [Review of *Teflon Flu on the Rise: What Doctors Need to Know About*]. *Docquity.com*. https://docquity.com/articles/teflon-flu-about-polymer-fume-fever/

O'Neill, G. J., Hollingsworth, A., Harbourne, N., & O'Riordan, E. D. (2019). Reducing stickiness in spray dried dairy emulsions. *Food Hydrocolloids*, *90*, 330–340. https://doi.org/10.1016/j.foodhyd.2018.12.033

Odegard, G. M. (2017). 6.2 Computational Multiscale Modeling – Nanoscale to Macroscale. *Elsevier EBooks*, 28–51. https://doi.org/10.1016/b978-0-12-803581-8.10021-9

Osborn, E. L. (2009). Casting aluminium cooking pots: labour, migration and artisan production in West Africa's informal sector, 1945–2005. *African Identities*, *7*(3), 373–386. https://doi.org/10.1080/14725840903031858

Ostendorf, F., Schmitz, C., Hirth, S., A Kühnle, Kolodziej, J. J., & Reichling, M. (2008). How flat is an air-cleaved mica surface? *Nanotechnology*, *19*(30), 305705–305705. https://doi.org/10.1088/0957-4484/19/30/305705

Pakhomova, A., Simonova, D., Koemets, I., Koemets, E., Aprilis, G., Bykov, M., Gorelova, L., Fedotenko, T., Prakapenka, V., & Dubrovinsky, L. (2020). Polymorphism of feldspars above 10 GPa. *Nature Communications*, *11*(1). https://doi.org/10.1038/s41467-020-16547-4

Patterson, W. (2009). *Basic Components and Procedures.* 1–52. https://www.sciencedirect.com/science/article/abs/pii/B9781893997912500079

Paul, N., Omah, A. D., Ezema, F. I., Iwuoha, E. I., & Nwanya, A. C. (2023). Silica extraction from rice husk: Comprehensive review and applications. *Hybrid Advances*, *4*, 100111–100111. https://doi.org/10.1016/j.hybadv.2023.100111

Pina, F. A., Malcherek, T., Angel, R. J., Carsten Paulmann, Jochen Schlüter, & Boriana Mihailova. (2018). Radiation-damaged zircon under high pressures. *Physics and Chemistry of Minerals*, *45*(10), 981–993. https://doi.org/10.1007/s00269-018-0978-6

Pittsburgh Supercomputing Center. (2024). GAUSSIAN [Review of *GAUSSIAN*]. *Pittsburgh Supercomputing Center*. https://www.psc.edu/resources/software/gaussian-2/

Poole, C. P., & Owens, F. J. (2003). *Introduction to nanotechnology*. John Wiley.

Poppe, L. J., Paskevich, V. F., Hathaway, J. C., & Blackwood, D. S. (2001). U. S. Geological Survey Open-File Report 01-041 - A Laboratory Manual for X-Ray

Powder Diffraction - KAOLINITE GROUP [Review of *U. S. Geological Survey Open-File Report 01-041 - A Laboratory Manual for X-Ray Powder Diffraction - KAOLINITE GROUP*]. In *U. S. Geological Survey*. U. S. Geological Survey. https://pubs.usgs.gov/of/2001/of01-041/htmldocs/clays/kaogr.htm

Poppe, L. J., Paskevich, V. F., Hathaway, J. C., & Blackwood, D. S. (2001). U. S. Geological Survey Open-File Report 01-041 - A Laboratory Manual for X-Ray Powder Diffraction - SMECTITE GROUP [Review of *U. S. Geological Survey Open-File Report 01-041 - A Laboratory Manual for X-Ray Powder Diffraction - SMECTITE GROUP*]. In *U. S. Geological Survey*. U. S. Geological Survey. https://pubs.usgs.gov/of/2001/of01-041/htmldocs/clays/smc.htm

Public Health. (2006). *Nanotechnologies: 1. What is nanotechnology?* Ec.europa.eu. https://ec.europa.eu/health/scientific_committees/opinions_layman/en/nanotechnologies/l-2/1-introduction.htm

Radnik, J., Mohr, C. H., & Claus, P. (2002). *On the origin of binding energy shifts of core levels of supported gold nanoparticles and dependence of pretreatment and material synthesis*. *5*(1), 172–177. https://doi.org/10.1039/b207290d

Ramachandran, K. I., Gopakumar, D., & Namboori, K. (2008). *Computational chemistry and molecular modeling : principles and applications*. Springer. https://doi.org/10.1007/978-3-540-77304-7

Ramachandran, K. I., Gopakumar, D., & Namboori, K. (2008). Semiempirical Methods [Review of *Semiempirical Methods*]. In *Computational Chemistry and Molecular Modeling* (pp. 139–154). Springer. https://link.springer.com/chapter/10.1007/978-3-540-77304-7_7#citeas

Ritme. (2025). Gaussian [Review of *Gaussian*]. *RITME Scientific Solutions*. https://ritme.com/en/software/gaussian/#:~:text=Complete%20studies%20of%20molecules%20and%20reactions%20It,the%20gaseous%2C%20liquid%20or%20solid%20(PCB)%20state.

Ribeiro, P., & de, R. (2014). Structural, electronic and elastic properties of $FeBO_3$(B = Ti, Sn, Si, Zr) ilmenite: a density functional theory study. *RSC Advances*, *4*(104), 59839–59846. https://doi.org/10.1039/c4ra11320a

Ruengcharungpong, S., Somjai, S., & Aeknarajindawat, N. (2019). CUSTOMER SATISFACTION AND BEHAVIOR OF USING NON-STICK COOKWARE PRODUCTS OF BANGKOK METROPOLITAN REGION. *INTERNATIONAL ACADEMIC MULTIDISCIPLINARY RESEARCH CONFERENCE in LOS ANGELES 2019*, 70–72. http://icbtsproceeding.ssru.ac.th/index.php/ICBTSLOSANGELES/article/view/392

Saikhwan, P., Geddert, T., Augustin, W., Scholl, S., Paterson, W. R., & Wilson, D. I. (2006). Effect of surface treatment on cleaning of a model food soil. *Surface and Coatings Technology*, *201*(3-4), 943–951. https://doi.org/10.1016/j.surfcoat.2006.01.021

Sajid, M., & Ilyas, M. (2017). PTFE-coated non-stick cookware and toxicity concerns: a perspective. *Environmental Science and Pollution Research*, *24*(30), 23436–23440. https://doi.org/10.1007/s11356-017-0095-y

Salo-Ahen, O. M. H., Alanko, I., Bhadane, R., Bonvin, A. M. J. J., Honorato, R. V., Hossain, S., Juffer, A. H., Kabedev, A., Lahtela-Kakkonen, M., Larsen, A. S., Lescrinier, E., Marimuthu, P., Mirza, M. U., Mustafa, G., Nunes-Alves, A., Pantsar, T., Saadabadi, A., Singaravelu, K., & Vanmeert, M. (2021). Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. *Processes*, *9*(1), 71. https://doi.org/10.3390/pr9010071

Samad, A., Baidya, S., Akhtar,U. S., Ahmed,K. S., Roy, S. C., & Islam, S. (2021). MANUFACTURE OF REFRACTORY BRICK FROM LOCALLY AVAILABLE RED CLAY BLENDED WITH WHITE PORTLAND CEMENT AND ITS PERFORMANCE EVALUATION. *International Journal of GEOMATE*, *20*(80). https://doi.org/10.21660/2021.80.j2033

Schaider, L. A., Balan, S. A., Blum, A., Andrews, D. Q., Strynar, M. J., Dickinson, M. E., Lunderberg, D. M., Lang, J. R., & Peaslee, G. F. (2017). Fluorinated Compounds in U.S. Fast Food Packaging. *Environmental Science & Technology Letters*, *4*(3), 105–111. https://doi.org/10.1021/acs.estlett.6b00435

Seneviratne, K., & Jayathilaka, N. (2016, January). *(PDF) Coconut Oil: Chemistry and Nutrition*. Research Gate. https://www.researchgate.net/publication/322818556_Coconut_Oil_Chemistry_and_Nutrition

Shamloo, E., Nickfar, F., Mahmoudzadeh, M., Sarafraz, M., Salari, A., Darroudi, M., Abdi-Moghadam, Z., Amiryosefi, M. R., Rezagholizade-Shirvan, A., & Rezaei, Z. (2023). Investigation of heavy metal release from variety cookware into food during cooking process. *International Journal of Environmental & Analytical Chemistry*, 1–17. https://doi.org/10.1080/03067319.2023.2192872

Sharma, A., & Joshi, S. C. (2023). Enhancement in fatigue performance of FRP composites with various fillers: A review. *Composite Structures*, *309*, 116724–116724. https://doi.org/10.1016/j.compstruct.2023.116724

Shikano, Y., Watanabe, H. C., Nakanishi, K. M., & Ohnishi, Y. (2021). Post-Hartree–Fock method in quantum chemistry for quantum computer. *The European Physical Journal Special Topics*, 230(4), 1037–1051. https://doi.org/10.1140/epjs/s11734-021-00087-z

Shimizu, T., Hamada, O., Sasaki, A., & Ikeda, M. (2012). Polymer fume fever. *Case Reports*, *2012*(dec09 1), bcr2012007790–bcr2012007790. https://doi.org/10.1136/bcr-2012-007790

Shon, H., Phuntsho, S., Okour, Y., Cho, D.L., Kim, K.S., Li, H., Na, S., Kim, J.B., & Kim, J., (2008). Visible Light Responsive Titanium Dioxide (TiO2). *J. Korean Ind. Eng. Chem*., 19 (1), https://www.cheric.org/PDF/KEHH/KH19/KH19-1-0001

Slobodian, M. R., Petahtegoose, J. D., Wallis, A. L., Levesque, D. C., & Merritt, T. J. S. (2021). The Effects of Essential and Non-Essential Metal Toxicity in the Drosophila melanogaster Insect Model: A Review. *Toxics*, *9*(10), 269. https://doi.org/10.3390/toxics9100269

Srinivasan, G. R., Sharma, Y., S Vijayalakshmi, & J Ranjitha. (2020). Computational analysis of triglyceride molecule involving in transesterification reaction. IOP Conference Series Materials Science and Engineering, 923(1), 012075–012075. https://doi.org/10.1088/1757-899x/923/1/012075

Statista. (2018). *Global vegetable oil consumption, 2018/19 | Statista*. Statista; Statista. https://www.statista.com/statistics/263937/vegetable-oils-global-consumption/

Tang, Z., Gui, X., & Fei, W. (2011). Utilization of Molecular Simulation Software Gaussian 03 to Design Absorbent for CO2 Capture. *Procedia Engineering*, *12*, 87–92. https://doi.org/10.1016/j.proeng.2011.05.015

Toth, R., Coslanich, A., Ferrone, M., Fermeglia, M., Pricl, S., Miertus, S., & Chiellini, E. (2004). Computer simulation of polypropylene/organoclay nanocomposites: characterization of atomic scale structure and prediction of binding energy. *Polymer*, *45*(23), 8075–8083. https://doi.org/10.1016/j.polymer.2004.09.025

Trivedi, J., Soni, B., & Rahim, S. M. (2017). CLAY-COOKWARE AND TABLE-WARE: OLD IS GOLD [Review of *CLAY-COOKWARE AND TABLE-WARE: OLD IS GOLD*]. *Management Journal of Siva Sivani Institute of Management*, *9*(2), 5–24. https://www.researchgate.net/publication/329238355

US Environmental Protection Agency (2018). *Fact Sheet: Draft Toxicity Assessments for GenX Chemicals and PFBS*. [online] *US Environmental Protection Agency*, Washington, D.C. : US Environmental Protection Agency, pp.1–6. Available at: https://www.epa.gov/sites/default/files/2018-11/documents/factsheet_pfbs-genx-toxicity_values_11.14.2018.pdf

Wang, Y., & Zhao, D. (2013). Size effect of gold nanoparticles on Au 4f7/2 binding energy in Au-bearing pyrite and arsenopyrite from Carlin-type gold deposit

[Review of *Size effect of gold nanoparticles on Au 4f7/2 binding energy in Au-bearing pyrite and arsenopyrite from Carlin-type gold deposit*]. *The SAO/NASA Astrophysics Data System*. American Geophysical Union, Fall Meeting 2013, abstract id. MR31A-2299

Weerakoon, D. (2013). Industry related mineral resources and the value addition process [Review of *Industry related mineral resources and the value addition process*]. *Vidurava*, *30*(1), 15–22. National Science Foundation. Colombo. https://dl.nsf.gov.lk/items/879c7273-c398-499b-a14b-7d638e62289e

Wieck, K. A. (2023). *Occurrence of Per- and Polyfluoroalkyl Substances (PFAS) in New Hampshire Biosolids*. University of New Hampshire Scholars Repository. https://scholars.unh.edu/honors/723

Wypych, G. (2021). *Handbook of Fillers*. Elsevier.

Yang, L. W., Rader, A. J., Liu, X., Jursa, C. J., Chen, S. C., Karimi, H. A., & Bahar, I. (2006). o GNM: online computation of structural dynamics using the Gaussian Network Model. *Nucleic Acids Research*, *34*(suppl_2), W24–W31. https://doi.org/10.1093/nar/gkl084

Yang, T., Hu, J., Li, T., Min, H., & Zhang, S. (2024). Molecular Energy of Metamorphic Coal and Methane Adsorption Based on Gaussian Simulation. *Processes*, *12*(12), 2621. https://doi.org/10.3390/pr12122621

Zhang, H., Ren, S., & Qiu, Y. (2023). Balancing the sustainable component of ethylene-vinyl acetate for achieved better compatibility improvement of wax-based warm mix additives in bitumen. *Colloids and Surfaces a Physicochemical and Engineering Aspects*, *675*, 132054–132054. https://doi.org/10.1016/j.colsurfa.2023.132054

Zhang, J., Soltani, A., Deng, A., & Jaksa, M. B. (2019). Mechanical behavior of micaceous clays. *Journal of Rock Mechanics and Geotechnical Engineering*, *11*(5), 1044–1054. https://doi.org/10.1016/j.jrmge.2019.04.001

Zucchini, A., Comodi, P., Nazzareni, S., & Hanfland, M. (2014). The effect of cation ordering and temperature on the high-pressure behaviour of dolomite. *Physics and Chemistry of Minerals*, *41*(10), 783–793. https://doi.org/10.1007/s00269-014-0691-z

APPENDICES

APPENDIX A

Industrial Survey Questionnaire on clay type utilization and potters' contribution on Clay pottery Industry in Gampaha District

1. Clay pottery making Center No:

2. Identification/name of clay pottery making center:

3. Gender Participation: Male ☐ Female ☐ Both Male and Female ☐

4. Clay Pottery Industry Type:

    a) medium-scale manufacturing centers ☐
    b) small-scale domestic manufacturing centers ☐
    c) Large-scale manufacturing centers ☐
    d) government sponsored clay-based creations village and training centers ☐

5. Clay types use for cooking pottery making

    a) Red Clay ☐
    b) Ball Clay ☐
    c) White Clay ☐

6. What is the pottery making process you use in your center?

    ………………………………………………………………………………………
    ………………………………………………………………………………………

7. What are the machines and instruments you use for pottery making in your center?

    ………………………………………………………………………………………
    ………………………………………………………………………………………

8. What type of clayware you make in your center?

    ………………………………………………………………………………………
    ………………………………………………………………………………………