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VOSviewer Application Analysis: Computational Physical Chemistry Case Study

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Abstract

Computational physics chemistry is a branch of chemistry which in its application uses the results of theoretical chemistry. It is then translated into a computer program to be able to calculate the properties of molecules and their changes. Computational chemistry can also simulate large systems such as liquids, gases, liquid crystals, and solids, then apply these programs to real chemical systems. The purpose of this research is to conduct a bibliometric analysis using computational physics chemistry as a case study by combining mapping analysis using VOSviewer software. The bibliometric and descriptive quantitative approach were applied in this research. The data obtained is a search result based on the keyword "computational physics chemistry" in Google Scholar. From the search results, 1000 articles published were found ranging from 2016-2021. The results show that computational physic chemistry research with term study was identified as the most studied in the 2016–2021 period. In conclusion, this study shows the importance of conducting a bibliometric analysis, especially in the field of computational physics chemistry. It is expected that this research can be a reference for future research in conducting and determining research themes.

Keywords: *Bibliometric, Computational Physical Chemistry, Data Analysis, VOSviewer*

1. Introduction

Computational chemistry is a branch of chemistry which in its process uses the results of theoretical chemistry, which are translated into computer programs to calculate the properties of molecules and the changes contained therein. Computational chemistry has the ability to simulate many molecules, such as proteins, gases, liquids, solids, and liquid crystals, and then apply these programs to real chemical systems. Examples of molecular properties that are calculated include atomic structure, energy and energy difference, charge, dipole moment, reactivity, frequency of vibration, and other spectroscopic quantities. Simulations of macromolecules and large systems may include studies of molecular conformation and changes thereof, phase changes, and forecasting of macroscopic properties based on behavior at the atomic and molecular level. In computer science and chemistry, the terms "computational chemistry" and "chemistry" are used interchangeably. As a result, computational chemists must be able to develop software to improve computers' ability to solve chemical problems, as well as convert computer-calculated data into data that can be visualized (such as molecular shapes) to make it easier for chemists to understand [1]. VOSviewer is bibliometric data mapping software or a data collection that displays bibliographic fields visually (title, author, author, journal, etc.). Bibliometric mapping software can provide us with a wealth of information and an overview of the evolution of science as well as the performance of research [2-4]. The word bibliography comes from the Greek words "bilio" (book) and "graphy" (writing). As a result, a bibliography can be defined as a list of books or articles on a particular topic [5-8]. VOSviewer software is useful for processing data related to data collection, formation, management, analysis, simulation, and so on [4]. Scientists can also find novelties in research using this software because it can represent a specific topic's impact. Furthermore, after entering data, this application is capable of detecting new trends, keywords, and the evolution of a specific topic frequency. Furthermore, VOSviewer software can be used to display bibliographic visualizations [6-7]. VOSviewer is used in the world of research for bibliometric analysis, looking for research areas that can still be researched and linked to get updates, as well as looking for library materials that are most widely used in the intended field. Many reports on computational physics have been published, including research by Myong. The study discusses the impact of computational physics on multi-scale [9]. Computational physics on graphics processing units was also done by Harju et al. They conducted the study because computational physics has been an essential part of personal computers for decades [10]. Many previous studies have discussed computational physics, but there have been few studies on bibliometric analysis in the field of computational physics research, particularly those that use VOSviewer software as a mapping analysis tool. This analysis is required to determine a term's quantity and timeliness. Furthermore, VOSviewer has been used in research in a variety of domains. Meng et al [11]. conducted a study with the theme of knowledge Atlas on the relationship between urban street space and residents' health, using VOSviewer as a computer program for bibliometric mapping. Meng et al. discovered 4552 published articles between 1999 and 2019. Similarly to the previous study, Li et al also conducted a study using the VOSviewer software application [12]. In their study, they used VOSviewer to determine which deep learning topic during 2007-2019 (Li et al). Meanwhile, Lin et al [13]. also conducts research on G20 countries on VOSviewer. However, in this study, we employed the most recent version of VOSviewer, 8.0.0, as well as computational physics and chemistry as case studies. This study provides a mapping tool that is not only confined to the trend of selected subjects, but also covers the evolution of a specific topic. Therefore, this research aims at conducting bibliometric analysis research in the field of computational physics chemistry by integrating mapping with VOSviewer software. It is because this analysis is important to determine the quantity and novelty of the data. It is hoped that this research can be a resource for academics in performing and deciding on research subjects, particularly those connected to computational physics chemistry.

2. Materials and methods

We used a qualitative descriptive method to describe the data used in this study. We gathered journal data, which is based on research from publications that have been published in Google Scholar-indexed journals. The journal data was related to computational physics chemistry. To gather the data, we used the reference manager application system as the reference, namely Publish or Perish. In this application, we can choose related articles or journals data from Crossref, Google Scholar, Google Scholar Profile, PubMed, Microsoft Academic, Scopus, and Web of Science. Publish or Perish is used to conduct a literature review of the chosen theme. Therefore, a similar research database was obtained. In this study, Google Scholar was chosen because it is free to use, as opposed to Scopus, which publishes or requires a subscription. The journals related to the chosen topic were discovered between 2017 and 2021, and 900 articles were discovered during that time period. The journal's criteria are that all journal data be indexed by Google Scholar and be relevant to the search for the themes needed in this study, which is bioenergy management. The information is then entered into VOSviewer. After being entered, the data is processed in order to match the desired or chosen keywords. VOSviewer then transformed the inputted data into an interconnected data map. In addition, we looked at the difference in the number of publications each year and classified the 10 articles with the most citations for each publisher out of a total of 1000 articles.

3. Results and Discussion

3.1. Research developments in the field of computational physics chemistry

Based on data obtained from a search using the Publish and Perish software, 1000 articles on the topic of Computational Physical Chemistry published in journals between 2017 and 2021 were discovered. Furthermore, based on articles published between 2017 and 2021, we categorized the articles with the most citations.

Table 1. Article Data in the Field of Climate Smart Agriculture

Cites	Title	Year	Publisher	Refs
1182	Catalysts and reaction pathways for the electrochemical reduction of carbon dioxide	2015	ACS Publications	[14]
1159	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table	2016	Wiley Online Library	[15]
911	Defining computational thinking for mathematics and science classrooms	2016	Springer	[16]
718	Computational 2D materials database: electronic structure of transition-metal dichalcogenides and oxides	2015	ACS Publications	[17]
417	The origin of ferroelectricity in Hf1−xZrxO2: A computational investigation and a surface energy model	2015	aip.scitation.org	[18]
331	Computational methods in drug discovery	2016	beilstein-journals.org	[19]
288	Machine learning for quantum mechanics in a nutshell	2015	Wiley Online Library	[20]
193	Cyber-physical-social system in intelligent transportation	2015	ieeexplore.ieee.org	[21]
183	Design of nanoparticle-based carriers for targeted drug delivery	2016	hindawi.com	[22]
161	Prediction carbon dioxide solubility in presence of various ionic liquids using computational intelligence approaches	2015	Elsevier	[23]

Table 1 displays the top 10 most cited articles in Computational Chemistry from various publishers with 1182 being the highest cites and 161 being the lowest cites.

3.2. Visualization computational physics chemistry topic area using VOSviewer

The maximum number of research topic keywords that can be linked to VosViewer is two. Following that, a data set of research articles was compiled in order to examine the relationship between the terms. The information gathered on the subject of bioenergy management was classified into seven groups, namely:

(i) Cluster 1 has 17 items: binding, catalyst, characterization, computational, computational design, computational screening, experimental, experimental study, impact, kinetic, ligand, metal organic framework, mof, number, performance, stability, and synthesis (See Figure 1).

(ii) Cluster 2 has 12 items: chemistry, computational chemistry, computational cost, computational model, computational resource, development, machine learning, model, prediction, quantum chemistry, review, and tool (See Figure 2).

(iii) Cluster 3 has 10 items: accuracy, case, comparison, computational efficiency, computational technique, dynamic, field, molecular dynamic, perspective, and range (See Figure 3).

(iv) Cluster 4 has 9 items: compound, density functional theory, derivative, dft, ionic liquid, light, mean, present study, and reactivity (See Figure 4).

(v) Cluster 5 has 4 items: cluster, electronic structure, level and theory (See Figure 5).

(vi) Cluster 6 has 3 items are adsorption, journal, and physical chemistry (See Figure 6).

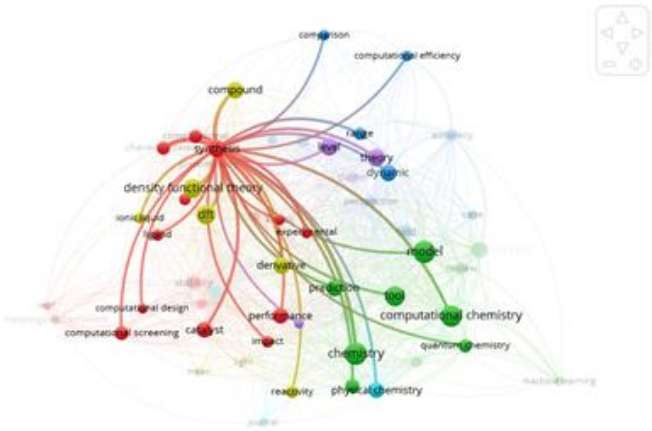

Figure 1. Cluster 1 Network visualization of Computational Physical Chemistry.

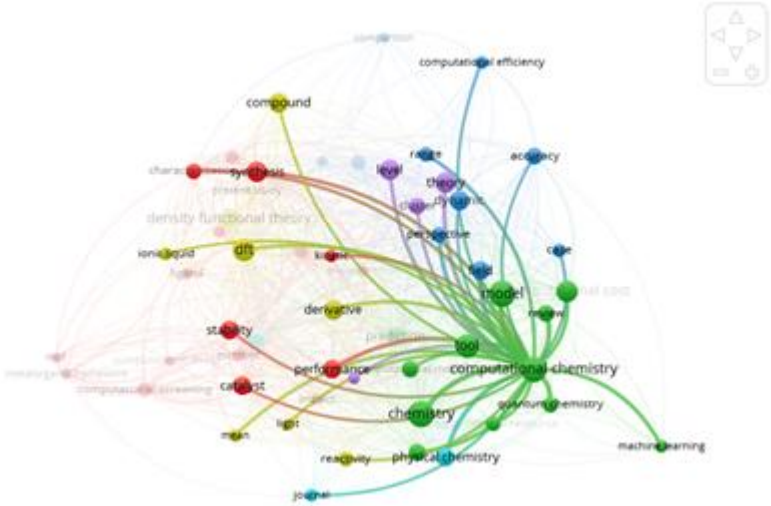

Figure 2. Cluster 2 Network visualization of Computational Physical Chemistry.

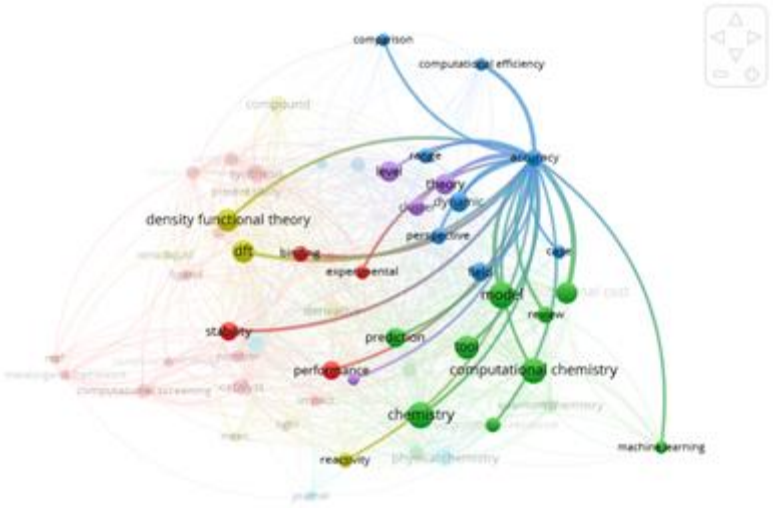

Figure 3. Cluster 3 Network visualization of Computational Physical Chemistry.

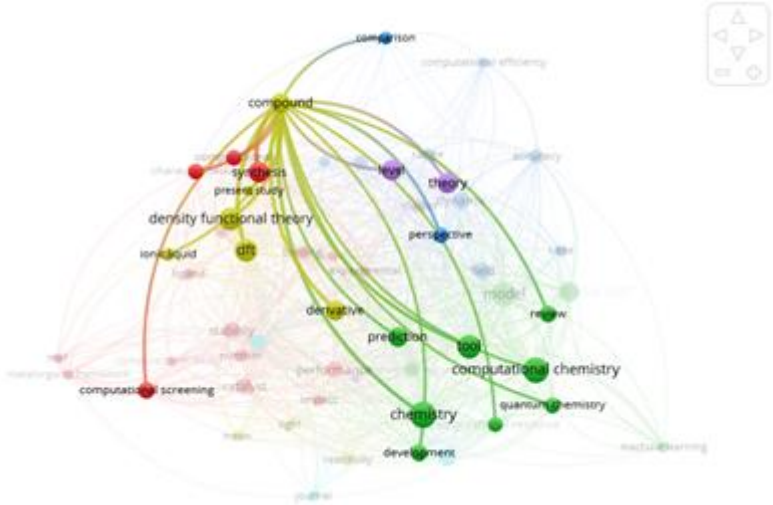

Figure 4. Cluster 4 Network visualization of Computational Physical Chemistry.

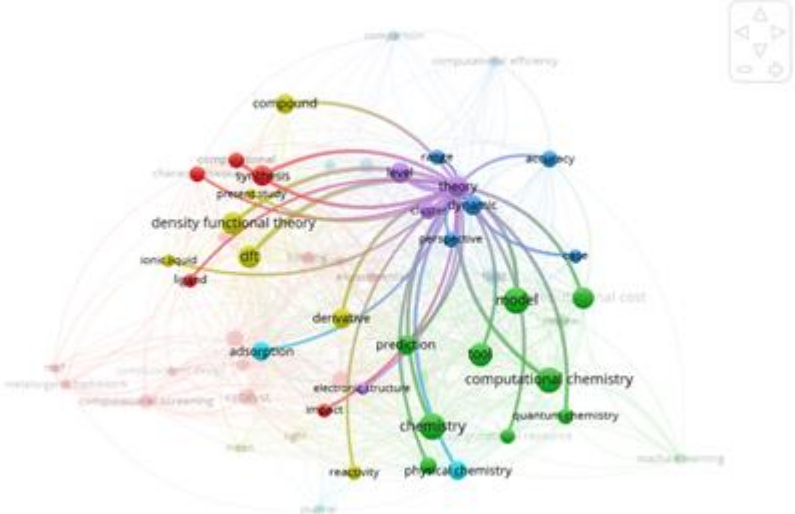

Figure 5. Cluster 5 Network visualization of Computational Physical Chemistry.

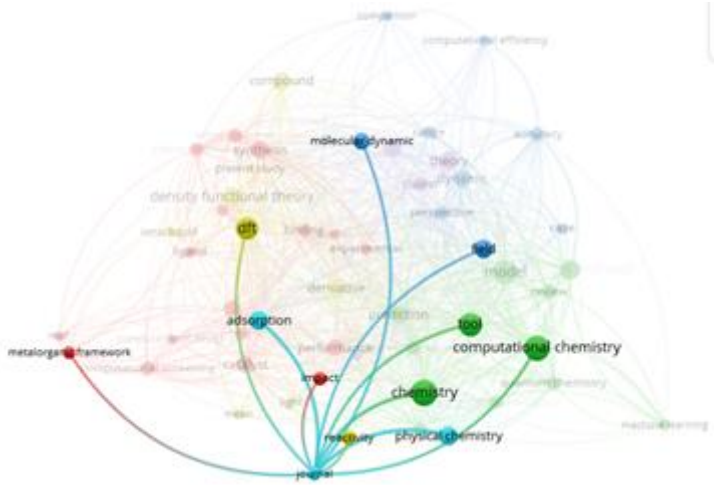

Figure 6. Cluster 6 Network visualization of Computational Physical Chemistry

3.3. Network visualization computational physical chemistry topic area using VOSviewer

In the VOSviewer application, term mapping is divided into three types, one of them is Network Visualization. On a map, Network Visualization depicts the relationships between terms [24-28]. Existing relationships are represented by networks or lines that connect one term to the next. Figure 7 depicts a Network Visualization of the term "Computational Physical Chemistry" from the VOSviewer application. Figure 7 depicts a description of each cluster within each of the investigated topic areas. Computational Physical Chemistry is included in cluster 2 with a total strength of 37 and an occurrence of 74, as shown in Figure 7. Computational Physical Chemistry is associated with Cluster 2, specifically the term chemistry. Meanwhile, the terms for Clusters 1, 3, 4, and 6 are synthesis, accuracy, compound, theory, and journal, respectively.

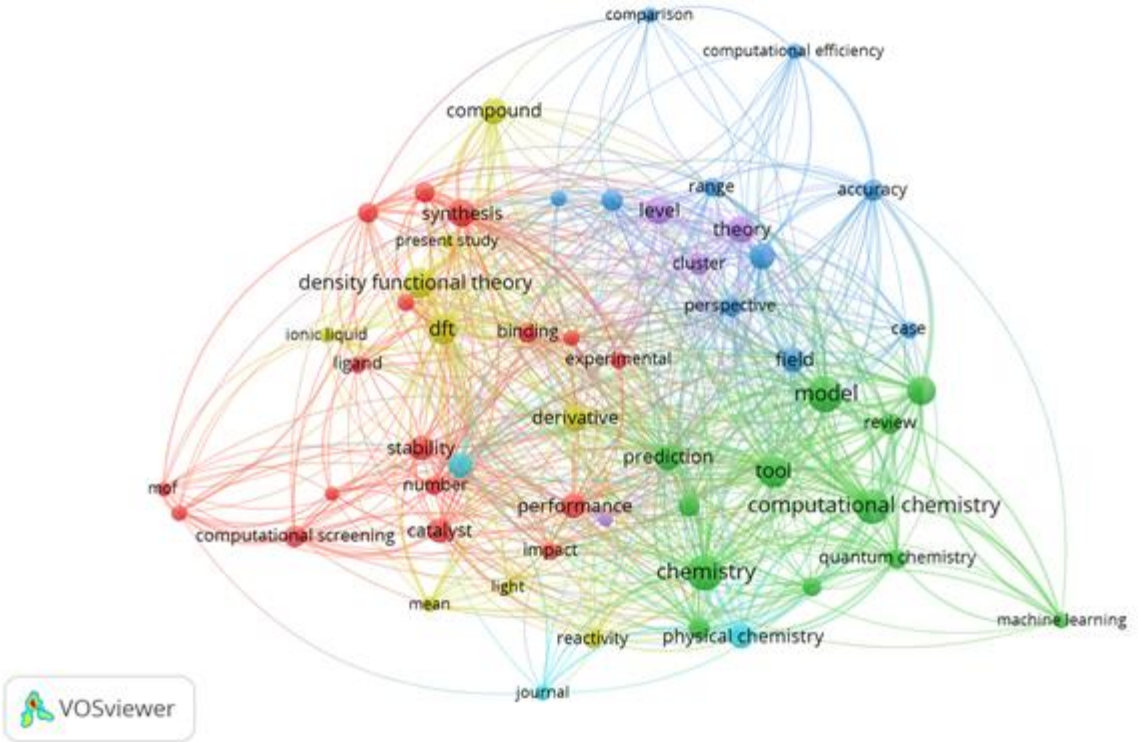

Figure 7. Network visualization of Computational Physical Chemistry

3.4. Overlay visualization computational physical chemistry topic area using VOSviewer

The VOSviewer application, in addition to Network Visualization, can display maps as overlays [29-33]. This mapping focuses on the level of term novelty in the research conducted. Figure 8 depicts the novelty of a term in Computational Physical Chemistry research. The mapping in the Overlay Visualization shows how popular a term is from year to year. Different colors in the Overlay Visualization indicate the renewal of a term within a certain time frame. We used the years 2016 to 2021 in this study. A darker color, closer to purple, indicates that the term was researched closer to 2016. While a lighter color closer to yellow is a term that has recently emerged from research.

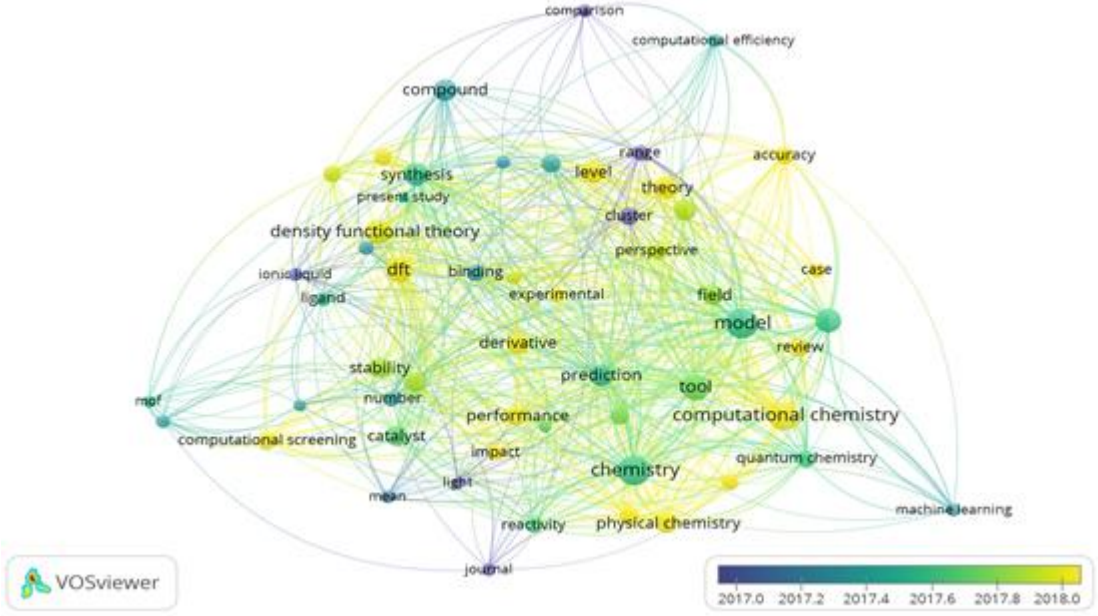

Figure 8. Overlay visualization of Computational Physical Chemistry.

Figure 8 shows an overlay visualization where Computational Physical Chemistry is the highest searched research keyword after chemistry and models. Computational Physical Chemistry is associated with 31 other terms. Terms related to the word Computational Physical Chemistry include machine learning, quantum chemistry, physical chemistry, case, journal, chemistry, reactivity, tool, model, review, case, field, performance, light, mean, catalyst, stability, derivative, perspective, dynamic, accuracy, theory, cluster, kinetic, dft, ionic liquid, level, range, computational efficiency, compound, and synthesis. Overlay visualization shows the relationship between terms and published articles years [34-39].

3.5. Density visualization computational physical chemistry topic area using VOSviewer

Density Visualization is one of mapping depictions in the VOSviewer application. Each term in this map will be divided based on its popularity in research. Figure 9 depicts density visualization in Computational Physical Chemistry. The color that appears in a term is used to demonstrate this type of mapping. The lighter the color appears, the more popular the research on the term becomes. On the other hand, as the color darkens or fades, research on the term becomes less frequent [40-44]. Figure 9 shows that there are several yellow tribes with a fairly large diameter. These terms are chemistry, computational chemistry, model, stability, theory and density functional theory. This means that these terms are terms that are often used in existing studies.

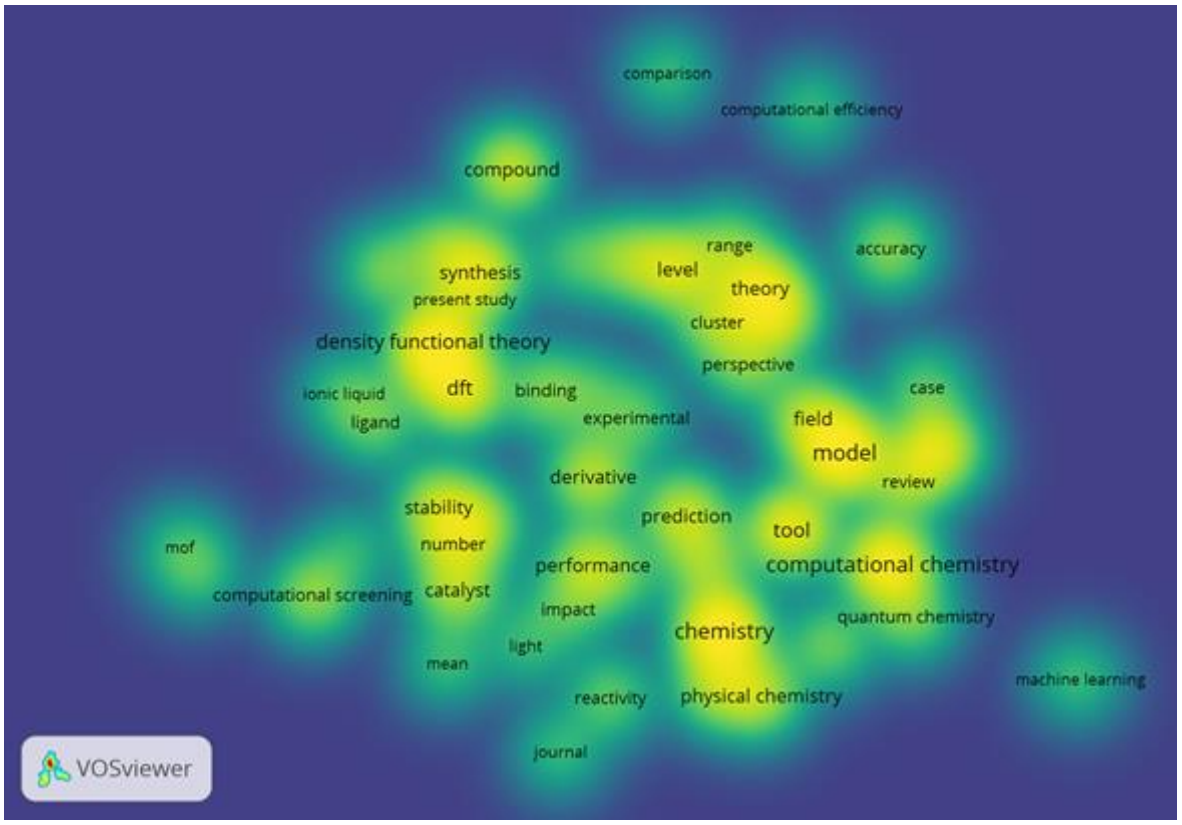

Figure 9. Density visualization of Computational Physical Chemistry

Figure 9 depicts a density map derived from an analysis of all articles published in Computational Physical Chemistry between 2016 and 2021. The density map depicts a yellow pattern in which the yellower the color, the larger the diameter of the circle and the denser the keywords. It implies that they appear more frequently, and the colors on the map fade or blend into the green background, implying that the keywords appear less frequently [45-47].

Conclusion

The purpose of this study was to examine the bibliometric literature in computational physics and chemistry. In this study, computational physics chemistry was divided into three categories, namely density functional theory, quantum chemistry, and model. In the search procedure, the keyword "computational physic chemistry" was used, which was based on a topic area with titles, keywords, and abstracts. As a result of the search, 1000 articles were found to be relevant. VOSviewer was then used to finish the mapping process and the top 10 papers with the most citations emerged from the search. Based on the results of analysis and mapping with VOSviewer, computational physic chemistry research with term study was identified as the most studied in the 2016–2021 period. Meanwhile, the bioenergy crop was the most researched in the field of bioenergy management.

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