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DFT and Docking Techniques: Bibliometric Analysis

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Abstract

The scientific use of Density Functional Theory (DFT) has expanded markedly, with >350,000 Scopus-indexed publications and ~30,000 articles in 2024 alone. Molecular docking has likewise grown (~177,600 records). When combined ("DFT AND docking"), we find 6,807 documents for 2010-2024. This study presents a bibliometric analysis of DFT + docking using Scopus and VOS viewer to quantify global output, identify prolific authors, journals, countries, and funders, and map collaboration and keyword structures that reveal where and how these in-silico approaches are applied. articles on Molecular docking, on the other hand, are a computational simulation technique for predicting the preferred orientation of a molecule (like a drug) when bound to a target receptor (like a protein), vital for understanding ligand-receptor interactions in drug discovery and design, reached about 180,000. When the two techniques are combined, production is limited to approximately 9,000 articles. Our objective is to gather the information on the combination of DF calculations with molecular dynamics via a bibliometric analysis using Scopus and VOS viewer to discuss the global production, the most published authors and countries, and the possible cooperation during the last decade.

Keywords: *Density Functional Theory (DFT); Molecular docking; Bibliometrics; Scopus; VOS viewer*

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1. Introduction

Density Functional Theory (DFT) is a computational quantum mechanical method used to predict the electronic structure, properties, and reactivity of molecules, offering insights into molecular stability and chemical behaviour (Zarrouk *et al.*, 2013; Gökce *et al.,* 2016; Merimi *et al.,* 2021; El-Demerdash *et al.,* 2023; Okoro *et al.,* 2025). DFT helps to understand reaction mechanisms, chemical stability, and how structural modifications affect a molecule's behaviour. It is also used to analyse and characterize newly synthesized compounds and to complete the interpretation of the experimental results, such as spectroscopic data (Avdović *et al.,* 2020; Miyah, 2022; Bouzammit *et al.,* 2025). Molecular docking is a computational simulation technique for predicting the preferred orientation of a molecule (like a drug) when bound to a target receptor (like a protein), vital for understanding ligand-receptor interactions in drug discovery and design (Agu *et al.,* 2023; Bouammali *et al.*, 2024; Toubi *et al.,* 2024). Together, these techniques provide a robust and integrated approach to drug design, enabling researchers to understand both the intrinsic properties of drug candidates and their interactions with biological targets. Importance of Density Functional Theory (DFT) in Predicting Molecular Properties:

DFT and molecular docking are complementary theoretical tools that support each other in the design of new cancer drugs (Leitzmann, 2016; Basaleh *et al.,* 2022; Er-rajy *et al.,* 2025; John *et al.,* 2025). In this way, we propose to regroup the articles on DFT and/or molecular docking through a bibliometric analysis using both Scopus analysis and VOS viewer over the last few decades.

2. Experimental work

2.1 Collection of data

Scopus offers a collection of data using several methods, including article title, abstract, keywords, author, first author, source title, affiliation (including name, city, or country), ISSN, and DOI. It also permits the analysis. The VOS viewer is another tool that provides more visibility into productive authors and countries via network, overlay, and density visualization, where authors and countries are represented by coloured circles, or nodes, linked by lines to indicate cooperation. VOS viewer is a free software tool for constructing and visualizing bibliometric networks from scientific literature (Orduña-Malea & Costas, 2021; N'diaye *et al.,* 2022; Bukar *et al.,* 2023; Tsilika*,* 2023; Hammouti *et al.,* 2025). Developed by researchers at Leiden University's Centre for Science and Technology Studies (CWTS), it is widely used in academic research to map the structure and trends of research fields (van Eck & Waltman*,* 2010).

3. Results and discussion

Scopus is a crucial tool for analysing data collected using one or more keywords within a given period. More than 317,000 articles were obtained when using "Density Functional Theory" from 1937 to 2024. **Figure 1** indicates the evolution of the progress of the number of articles over time. A notable increase in the number of articles was observed from 1995, reaching 30,900. When "molecular docking" is used, 177,600 articles are received on Scopus. A total of 6807 articles were gathered from 2010 to 2024 using the terms "DFT and Docking", and **Figure 2** shows the progress of articles from 2010 to 2024.

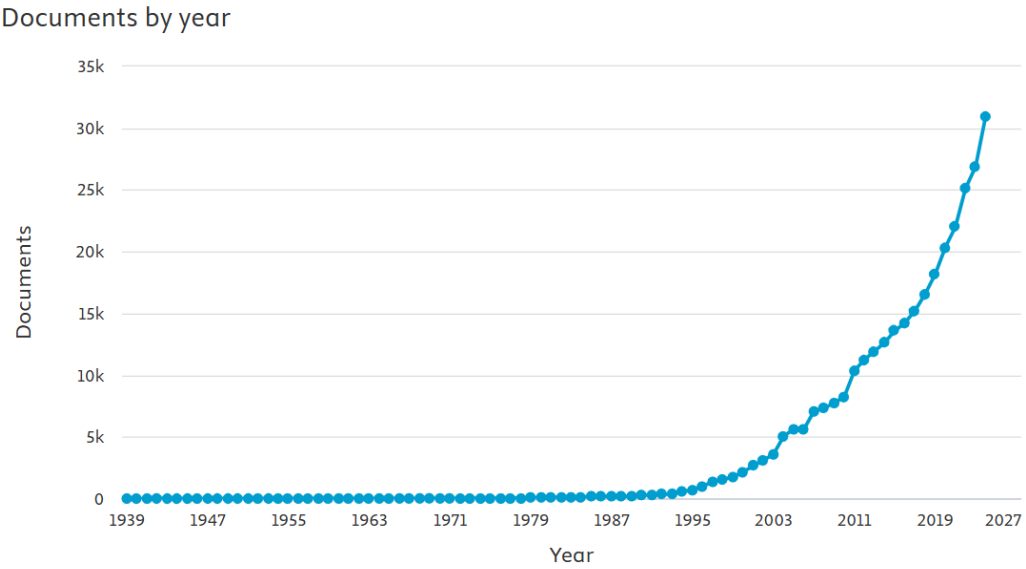

Figure 1. Produced documents on "Density Functional Theory" from 1937 to 2024 (Scopus).

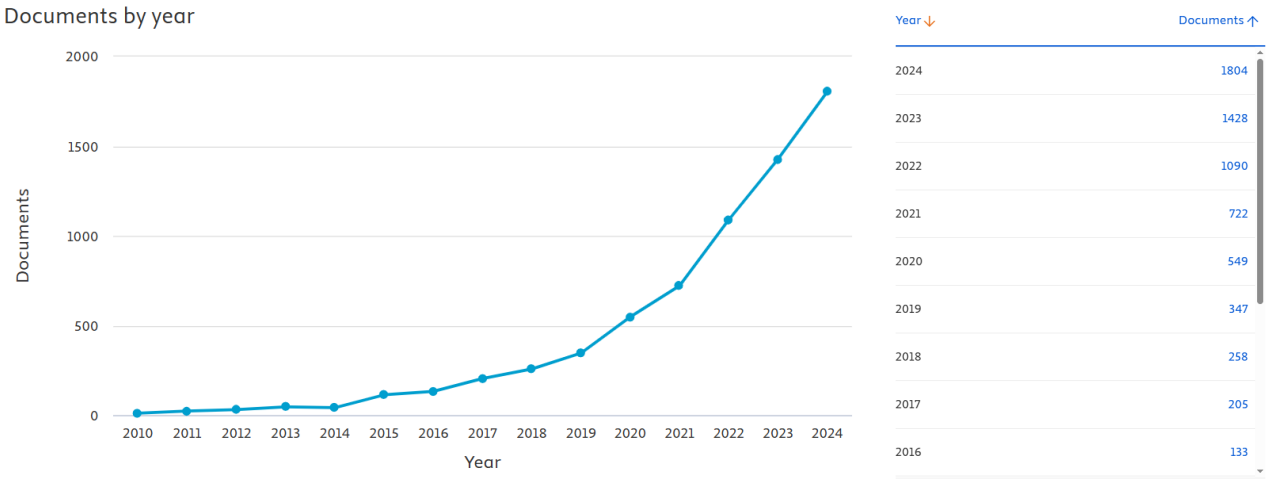

Figure 2: Year-wise publication of bibliometric papers "DFT & Docking" (2010 – 2024)

More than 1800 papers were recorded in 2024. 96.4% of the production is research articles, i.e., 6561 articles, and less than 3% are conference papers, reviews, or Data papers (**Figure 3**). As described above, DFT and molecular docking are highly supportive theoretical tools in various fields, including

Chemistry, Materials Science, Physics, Chemical Engineering, Pharmacology, and Medicine, as illustrated in **Figure 4**. The most published authors are ranked as in **Figure 5**, Muthu S. reaching 228 articles, occupying the head of this list, followed by Luis H. with 98 articles, Thomas R. (89), Javed S. (82), Mary Y.S. **(77) …** Scopus Analysis indicates also that India is the most prolific country (3107 articles); this reflects the Indian investment in Mathematics and Computer Science (**Figure 6**). In second position, Saudi Arabia confirms the scientific and technological progress as an emergent country (1377 articles), followed by Egypt, Turkey, China etc. These findings are supported by the list of Funding Sponsors, where the "Department of Science and Technology, Ministry of Science and Technology, India" is at the top of the list (**Figure 7**), and King Saud University is in second position, as indicated in its country (**Figure 6**).

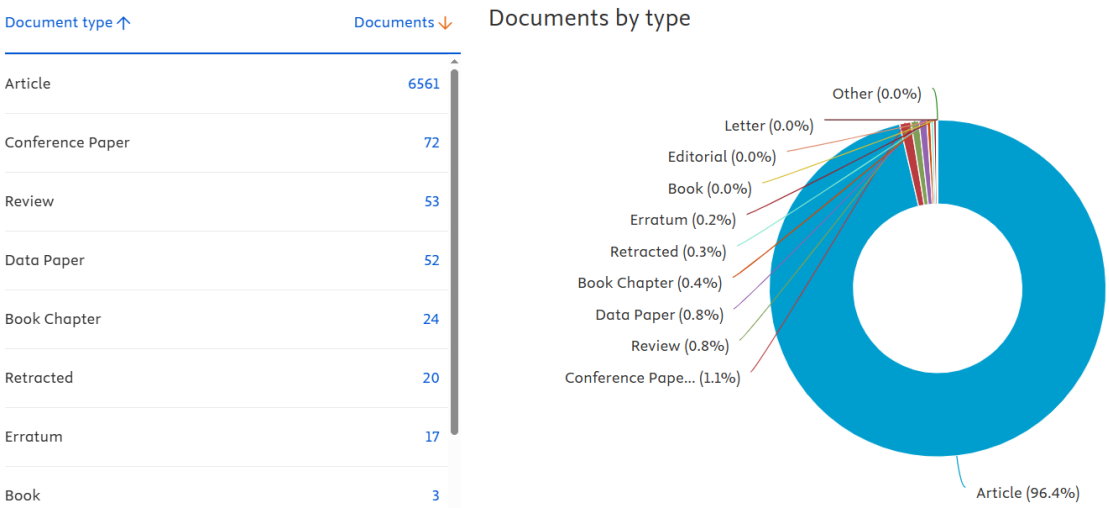

Figure 3: repartition of articles by type

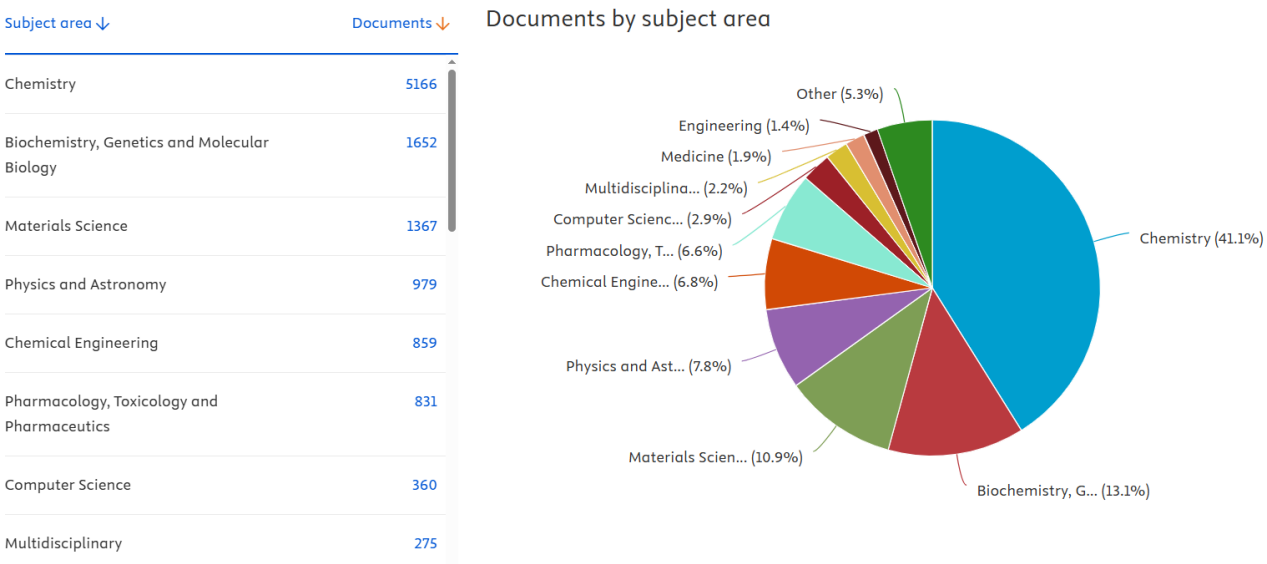

Figure 4: repartition of articles by area

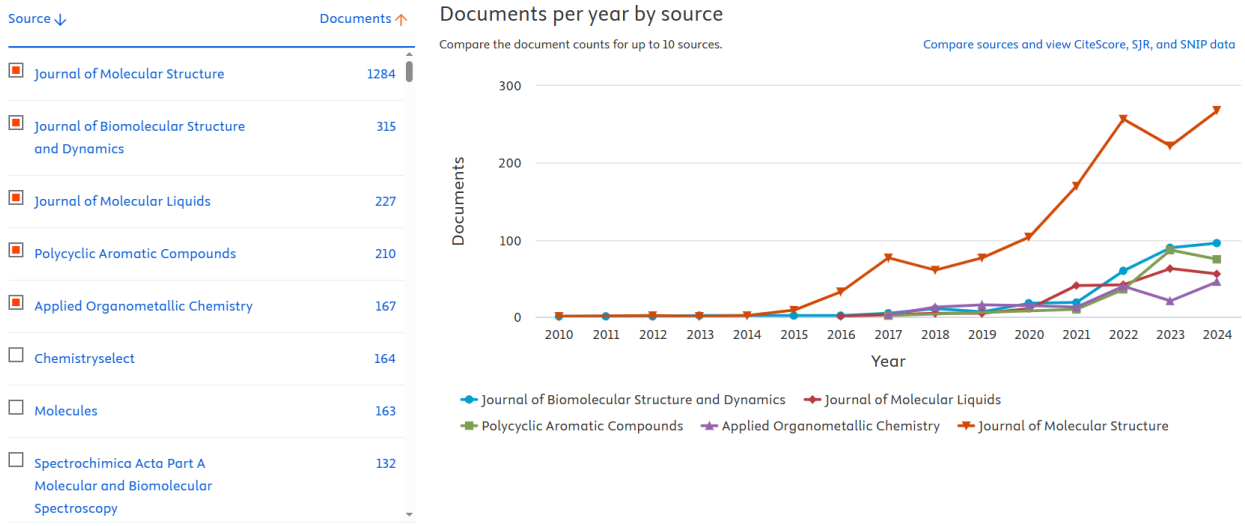

Figure 5: Most journals preferred by the authors

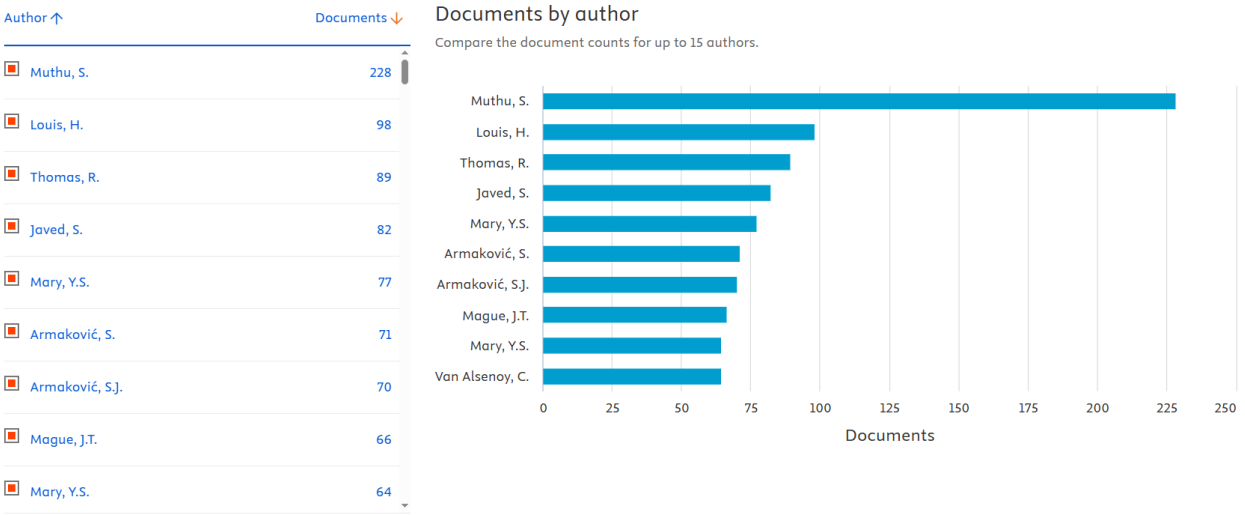

Figure 5: Most profiled authors

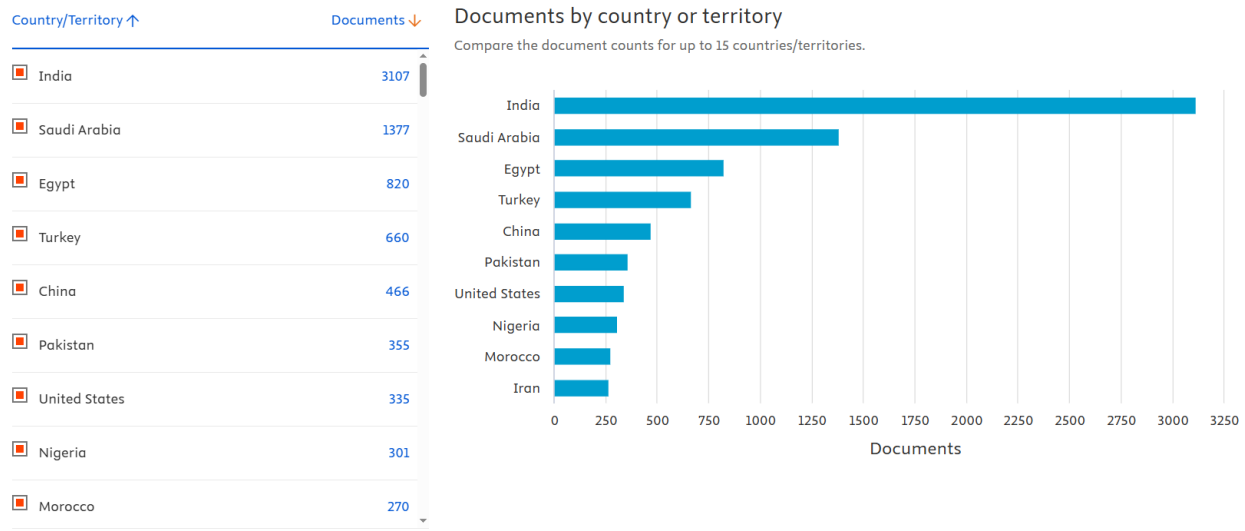

Figure 6: ten most concerned countries

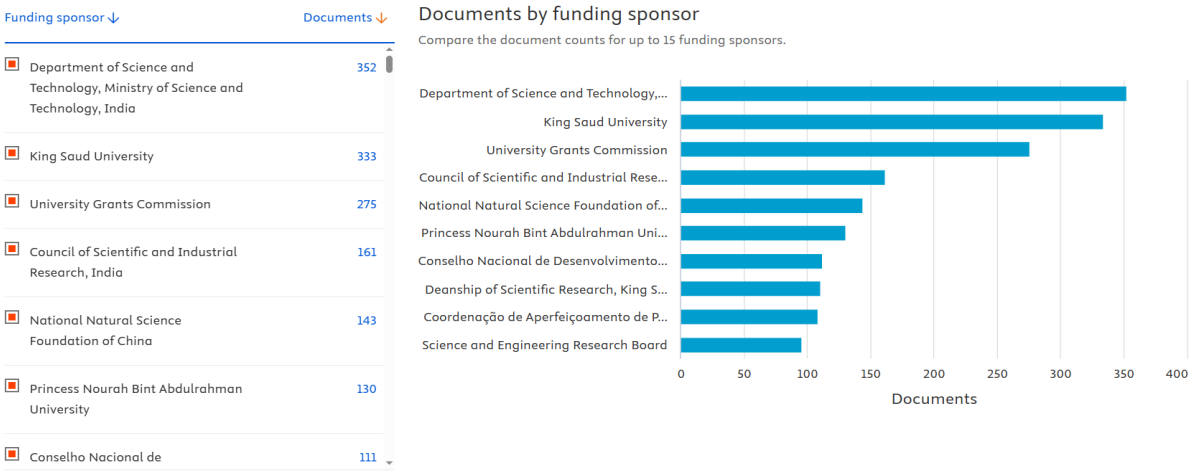

Figure 6: The ten most funding institutions for research in this area.

This result can be consolidated by VOS viewer by using the Scopus data connecting authors or countries. 2,538 authors from 129 countries published 6,807 articles, but only 2,026 authors have at least five articles. Coloured nodes indicate the mentioned authors. The largest mustard node is attributed to the best researcher, Muthu from India, who has a total of 411 articles, an H-index of 56, and 9,656 citations. The second brown node for the Nigerian Louis Hitler (2nd), and the third one is also Indian: Thomas Renjith (Grey node). A light pink node indicates the Indian Javed Saleem (4th), etc (**Figure 7**).

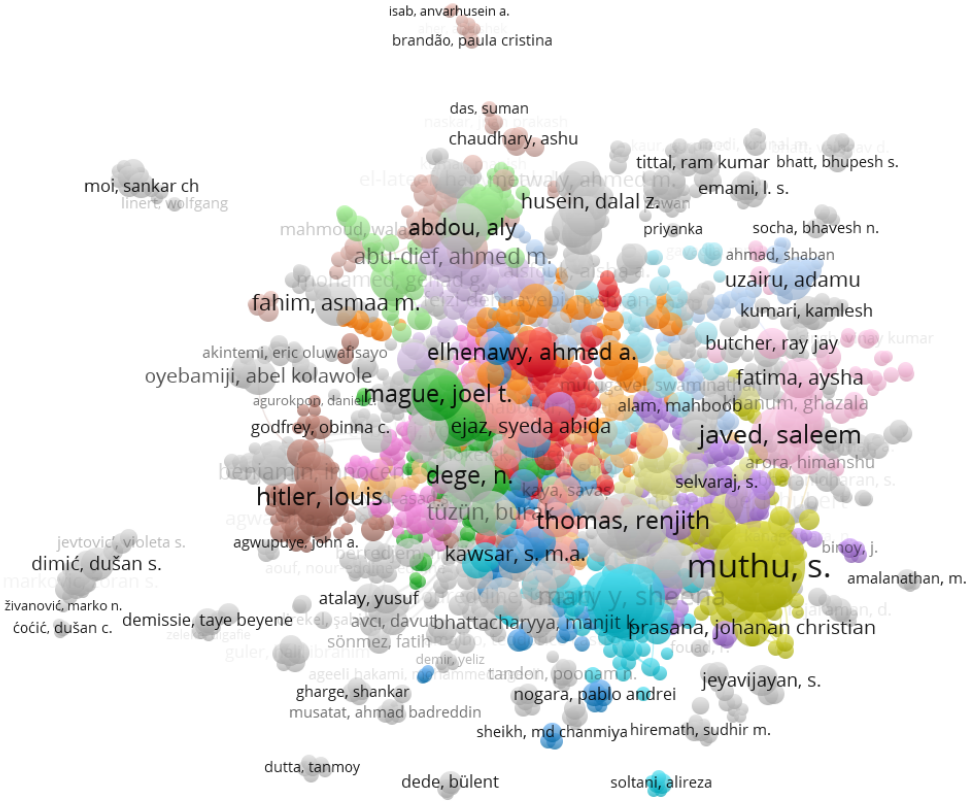

Figure 7: Network visualisation of the authors

The VOS viewer overlay visualization presentation provides additional information about the publication dates (Nandiyanto & AL Husaeni, 2022; Saiz-Alvarez, 2024; Gandasari *et al.,* 2024). Authors with dark blue nodes are active around 2020, and those with light yellow nodes have published at present (**Figure 8**).

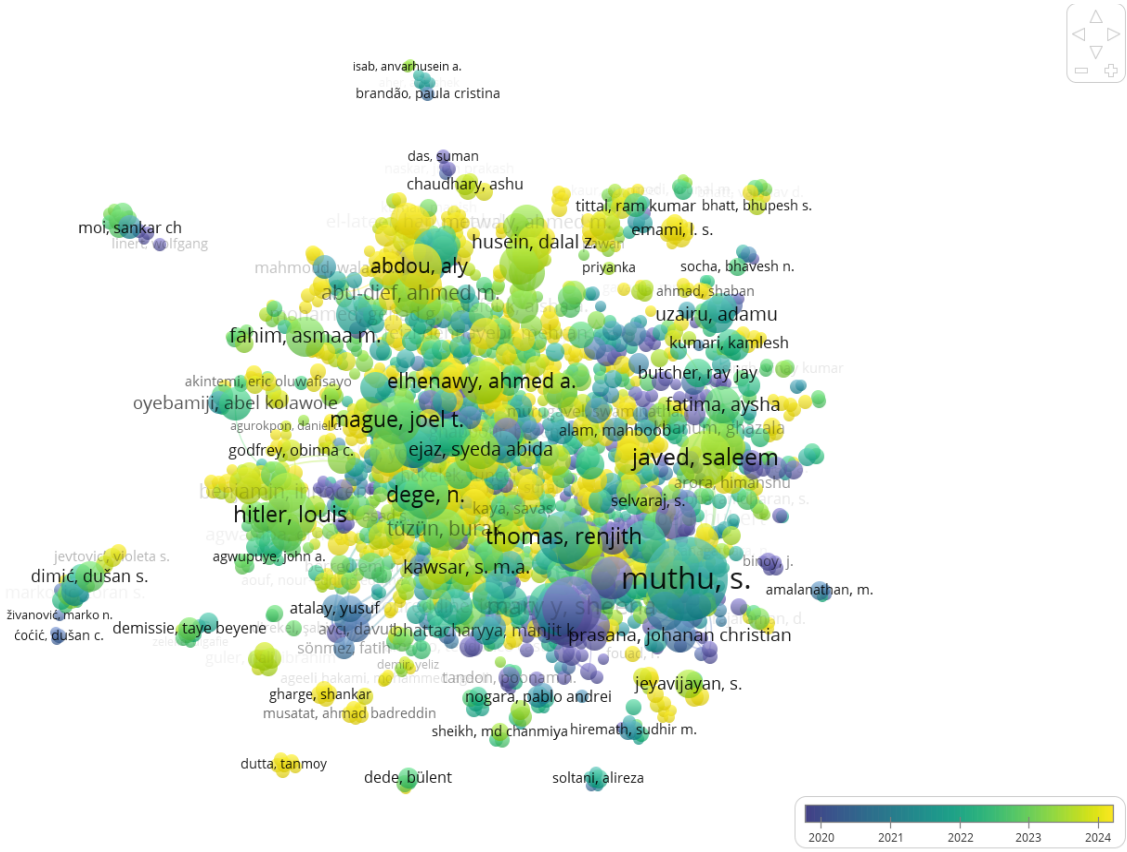

Figure 8: Overlay visualisation of the authors (VOS viewer)

Density Visualization is one of the mapping depictions in the VOS viewer application. **Figure 9** depicts the density visualization of authors. The colour used in a term is employed to illustrate the most prolific authors by using a lighter shade of yellow. The colour darkens indicates that the author's research is less frequent (Ullah, 2023; Laita *et al.,* 2024; Kachbou *et al.,* 2025).

Figure 10 shows that there are several coloured nodes related to the collected countries. The brown node is attributed to India, with the largest diameter. A purple node shows Saudi Arabia, and all the others are listed in **Figure 6. Figure 11** shows the interest of countries, both recent and earlier. For example, the light green node indicates that India contributed recently, while the yellow nodes are from around 2024 and earlier than 2021. The presentation of density visualization suggests that India is the most published country, marked with a yellow colour.

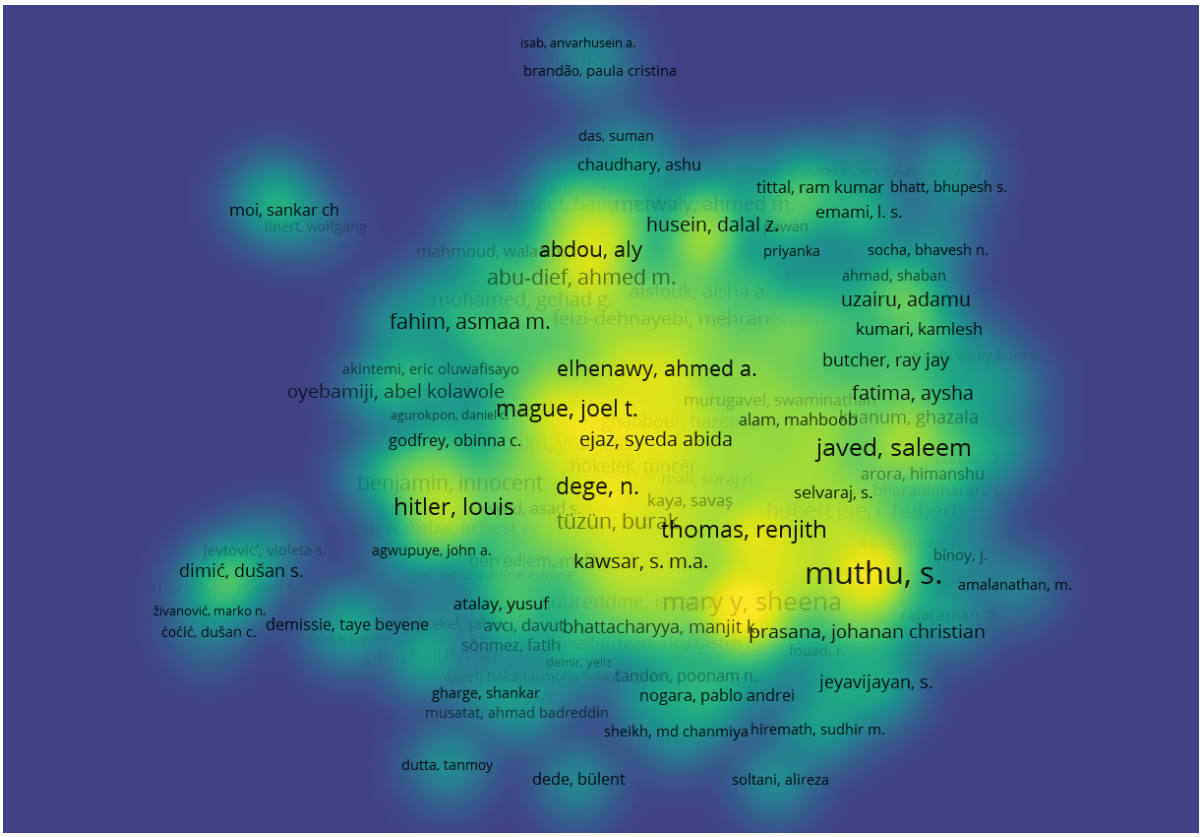

Figure 9: Density visualisation of the authors (VOS viewer)

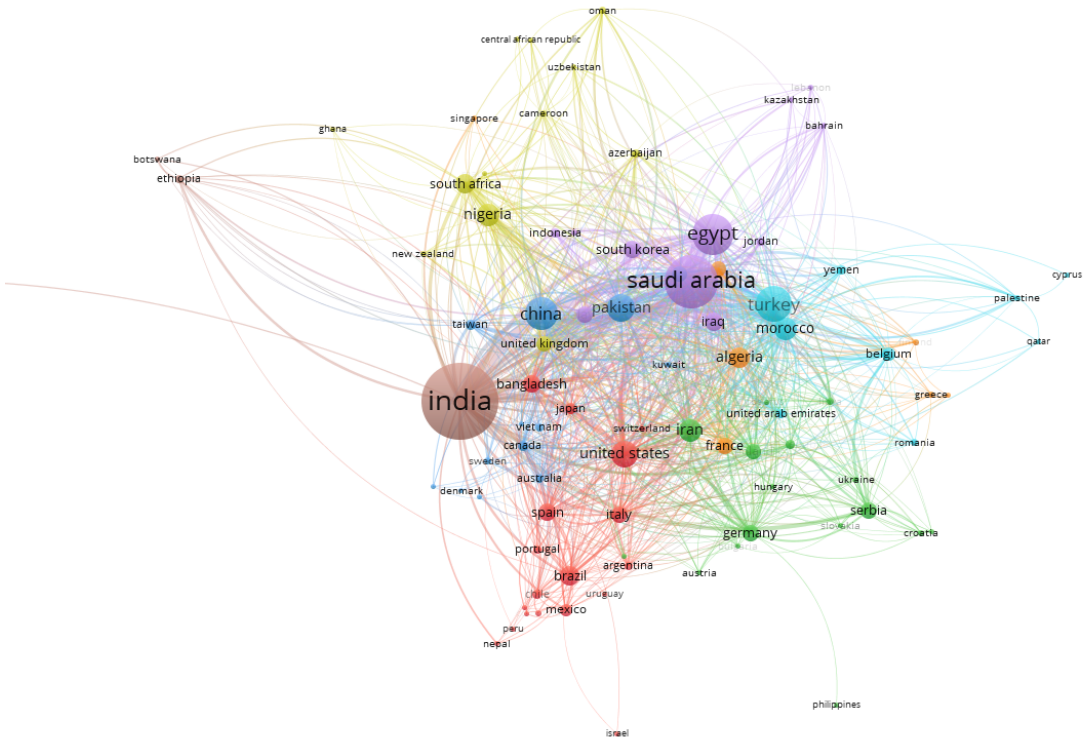

Figure 10: Overlay visualisation of the 90 countries (VOS viewer)

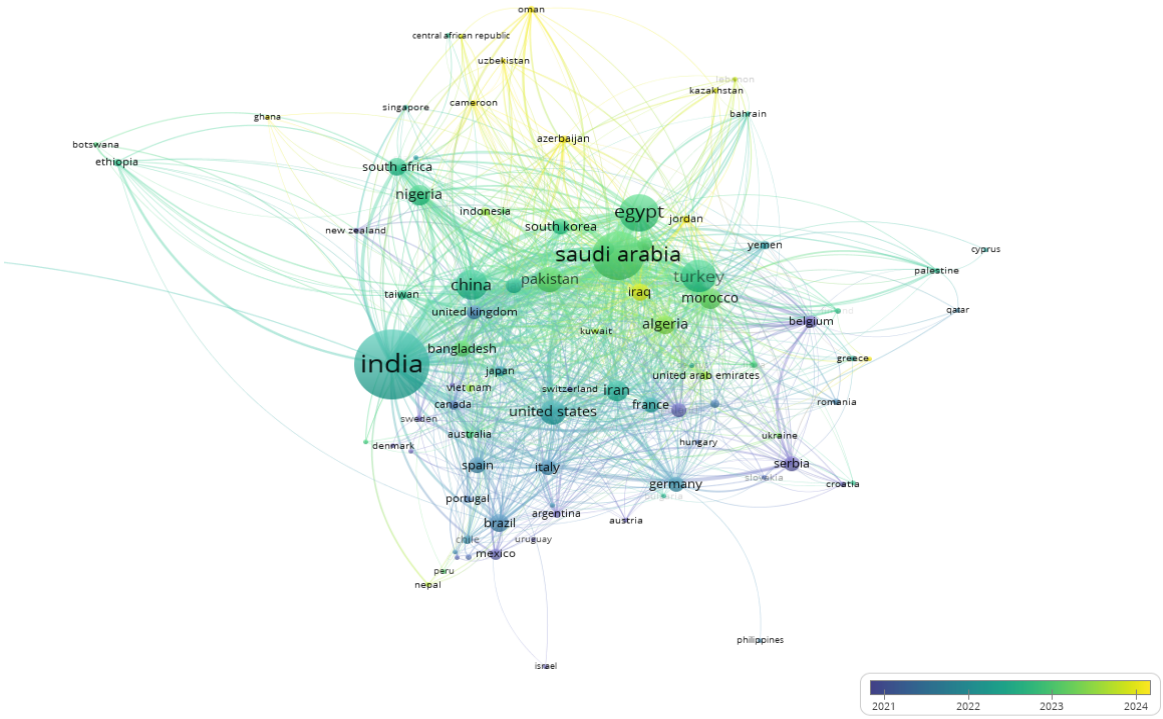

Figure 11: Overlay visualisation of the 90 countries (VOS viewer)

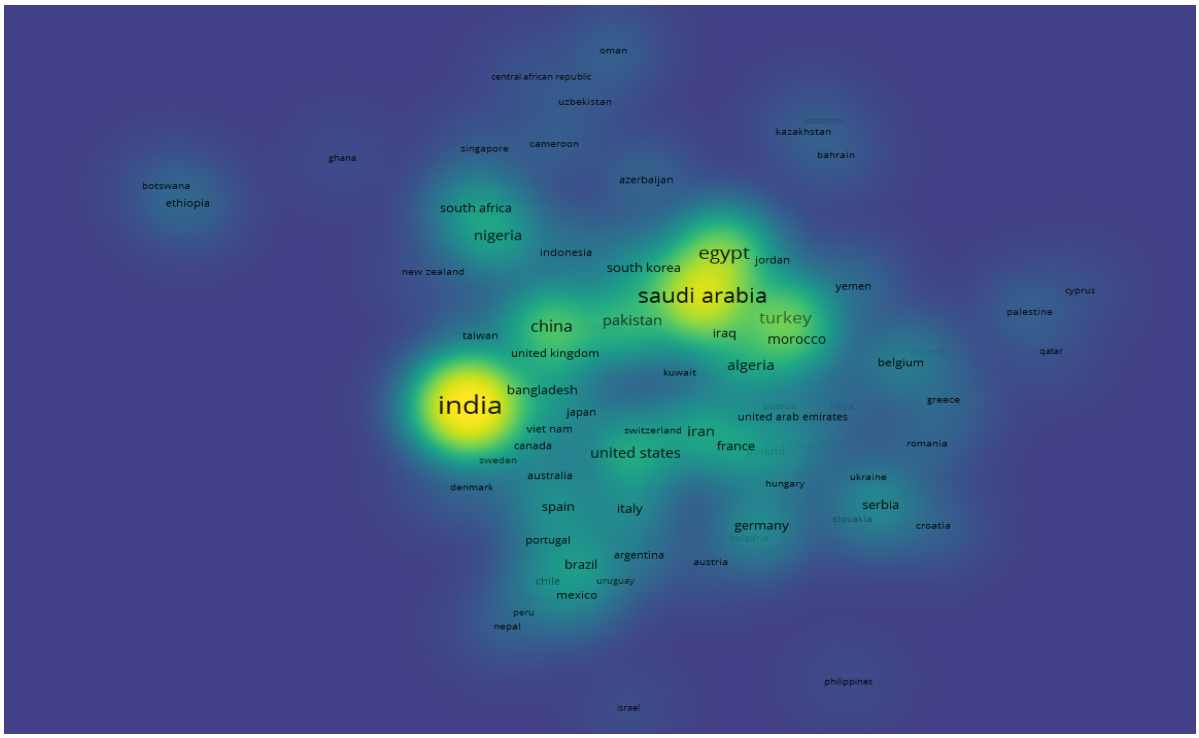

Figure 12: Density visualisation of the 90 countries (VOS viewer)

Conclusion

By consolidating the Scopus record of DFT (>317k documents) and molecular docking (~177.6k documents) with the 6,807 “DFT AND docking” publications from 2010–2024, this study shows that the joint use of quantum-level electronic structure methods and target-level binding models has moved

from niche practice to a mainstream, rapidly accelerating in-silico strategy (with >1,800 items in 2024; research articles ~96.4%). VOS viewer maps reveal concentrated yet expanding author and country clusters, with strong contributions from India, Saudi Arabia, and an increasingly diversified global network. Conceptually, coupling DFT with docking provides a mesoscale bridge from molecular reactivity and stability to protein-ligand recognition that enables more informed hypothesis generation, prioritization of candidates, and mechanism-aware interpretation across chemistry, materials, and biomedicine. Methodologically, this corpus also underscores the need for standardized search strings and reporting (queries, thresholds, software versions), curated author/affiliation disambiguation, and transparent, reproducible pipelines linking bibliometrics to scientific insight. Looking ahead, a next phase should integrate co-citation and longitudinal keyword-evolution analyses with multiscale modeling (e.g., DFT → docking → MD and AI-assisted scoring) and outcome-grounded validation against experimental benchmarks. Such a program would convert bibliometric structure into actionable guidance for discovery, accelerating the design–make–test–learn cycle while maintaining rigor, traceability, and domain relevance.

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Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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