عنوان مقاله:

Unleashing the Potential of Machine Learning in Chalcogen Bonding Research

محل انتشار:

فصلنامه علم و فناوری اوراسیا, دوره 4, شماره 2 (سال: 1403)

تعداد صفحات اصل مقاله: 32

نویسندگان:

Department of Chemical Sciences, Federal University Wukari, Taraba State, Nigeria - - -

Department of Chemistry, Rivers State University, Nkpolu-Oroworukwo, Port Harcourt, Nigeria - - -

Department of Chemical Sciences, Federal University Wukari, Taraba State, Nigeria - - -

خلاصه مقاله:

Chalcogen bonding, a non-covalent interaction involving chalcogen atoms (e.g., sulfur, selenium, and tellurium), plays a crucial role in various chemical and biological processes. Understanding and characterizing chalcogen bonding interactions are essential for designing novel materials, medications, and catalysts. In recent years, machine learning has emerged as a powerful tool for studying molecular interactions, including chalcogen bonding. This study provides an overview of the application of machine learning in characterizing chalcogen bonding. Experimental techniques, such as infrared (IR), nuclear magnetic resonance (NMR) spectroscopy, and X-ray crystallography, have been used to study chalcogen bonding. However, these methods often suffer from inherent experimental challenges. On the other hand, computational approaches, including quantum mechanics (QM) and molecular dynamics (MD) simulations, offer valuable insights into the electronic structure and energetics of chalcogen bonding. Nonetheless, they can be computationally demanding and may not fully encompass the diversity of chalcogen bonding interactions. Machine learning, with its ability to identify patterns and relationships in vast datasets, presents a promising alternative for characterizing chalcogen bonding. The study explains how machine learning algorithms, such as supervised and unsupervised learning, can be employed to classify and predict chalcogen-bonded complexes using neural network potentials to assess the persistence of chalcogen bonds in solution and ML models to predict two key solid-state synthesis conditions that must be specified for chalcogenide glasses. By integrating experimental data and computational results, machine learning models offer a holistic approach to understanding chalcogen bonding in various molecular systems. It emphasizes the integration of experimental and computational data as a means to maximize the accuracy and applicability of machine learning models and envisions a promising future for machine learning in characterizing chalcogen bonding interactions.

کلمات کلیدی:

Chalcogen bonding, Non-covalent interactions, Machine Learning, Artificial intelligence