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Machine learning approach to map the thermal conductivity of over 2,000 neoteric solvents for green energy storage applications

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ABSTRACT

Interest in green neoteric solvents, such as ionic liquids (ILs) and deep eutectic solvents (DESs), has increased dramatically in recent years due to their highly tunable properties. One application that has stimulated many experimental studies is their use as green solvents in energy and heat storage. Nevertheless, their theoretically infinite chemical space hinders their practical application and makes it impossible to conclude universal laws regarding their feasibility. Herein, for the first time, we combine molecular modeling and machine learning (ML) to develop a holistic tool that can map the thermal conductivity space of both ILs and DESs to bring their use as green solvents into industrial reality. Two molecular representations were used: the σ-profiles (σ_p) and the critical properties (CPs). In addition, six ML algorithms were evaluated, and the results showed that artificial neural networks (ANNs) demonstrated fast and accurate predictions of the thermal conductivity space with R^2 values of 0.995 and 0.991 using σ_p and CPs, respectively. The ANNs were further experimentally validated by additional measurements of 5 ILs and 5 DESs, which have not been previously reported in the literature. The results showed an excellent agreement, with deviations of only 2.82% and 2.71% using σ_p and CPs, respectively. Subsequently, the ANNs were used to successfully screen 1,156 ILs and 1,125 DESs to demonstrate a guided molecular design to achieve different thermal conductivity values. The proposed ANNs were also loaded into an easy-to-use spreadsheet included in the Supplementary materials. This work showcases the power of data-centric modeling for predicting the chemical spaces of ILs and DESs to promote their use as green solvents for various potential applications, including energy storage, fuel cells, and carbon dioxide capture.

1. Introduction

The scientific community, both academic and industrial, attaches great importance to the introduction of green approaches and technologies and advocates their integration into various processes. This notion has also been instilled by the principles of Green Chemistry [1], which promote the careful design of processes with particular attention to

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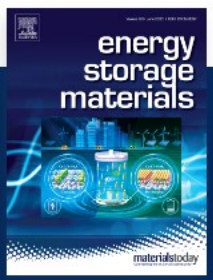

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