Abstract

The growing demand for sustainable energy solutions has heightened the quest for efficient energy storage materials. Indeed, renewable energy sources such as solar and wind need reliable energy storage systems – usually based upon advanced and innovative materials – able to harness and distribute such intermittent energy. However, the traditional *Edisonian* trial-and-error approach is time-consuming, expensive, and often limited in scope. Within this context, it is thus not a surprise that Artificial Intelligence (AI) is standing out as a powerful tool for accelerating materials discovery. In such a framework, this thesis focuses on the exploitation of AI capabilities in order to speed up the identification and characterization of materials for selected energy storage applications, with the final aim of facilitating the development of more efficient and sustainable energy storage technologies.

Specifically, the thesis is organized into several sections, each devoted to different applications of AI in the realm of energy storage, with a focus on Metal-Organic Frameworks (MOFs) , superconductors, and solar fuels. Through a comprehensive analysis, it demonstrates how AI methodologies can enhance the material discovery process, from initial data collection to the final optimization of properties.

First, this work focuses on AI and MOFs, and particularly on their role in low temperature seasonal water-sorption thermal energy storage. It investigates the physical properties of MOFs and describes how AI can be used to identify and optimize descriptors (i.e., material features) for MOF sorption properties. Also, the thesis discusses the challenge of creating an efficient protocol that can handle the variability of adsorption properties in the entire isosteric field of different MOF-H_2O working pairs with only little access to it.

Second, it deals with the application of AI in the field of superconducting materials. It outlines the process of dataset creation, the selection of appropriate regression models and descriptors, their analytical mixing, and the use of both entropy-based and traditional binary classifiers to identify new potential superconductors. It also addresses various data quality issues, such as bias, about the reliability of predictive models and proposes a methodology to assess and circumvent it in materials discovery. This allows to pinpoint, with a reasonable degree of reliability, interesting materials worth of further investigation over a recently published database comprising nearly 400,000 AI-generated stable materials.

Finally, it examines the use of AI in optimizing solar fuel production by means of a photocatalytic system. In this regard, it demonstrates how Bayesian Optimization can be effectively utilized to navigate a five-dimensional parameter space, steering a

campaign of approximately 100 experiments towards a comprehensive holistic optimum that balances multiple performance metrics. Also, it points out the application of post-optimization analysis over the data harvested during such experimental campaign to get more insight into the chemical behaviour of the system. Finally, employing the mixing features algorithm developed for superconductors, predicts alternative configurations that use a lower amount of the most valuable components, without compromising the overall performance.

Remarkably, the AI methods discussed in this thesis are blessed by generality and, as such, are applicable to a broader range of materials and storage technologies. Also, integrating more advanced techniques, such as transfer learning, may further increase the prediction accuracy and the discovery rate, potentially overriding many costly simulations/experiments still currently indispensable.