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The Most Effective Virtual Screening Pathway for Choosing Redox Active Organic Compounds

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Abstract

The urgent demand for creating novel energy storage technologies based on organic electrode materials that can improve upon the limitations of the current lithium ion batteries has grown along with the global interest in renewable energy. Finding materials whose Redox Potential (RP) satisfies certain design goals is a crucial issue for this endeavour. Using a High Throughput Virtual Screening (HTVS) pipeline that permits quick screening of organic compounds that meet the relevant requirements, we offer a computational approach in this study to address this difficulty. We demonstrate how a collection of surrogate models with various levels of accuracy and complexity may be used, starting from a high fidelity model for calculating the RP of a particular material.

***Keywords:** Frustrated Lewis pairs; catalytic hydrogenation; Water tolerance; Reductive amination; Redox Potential (RP)*

Introduction

The urgent need to create unique energy storage systems that can get around the practical limitations of traditional Li ion batteries has arisen from the growing interest in renewable energy sources. Particularly, organic electrode material based energy storage systems have drawn more interest as a result of a variety of advantageous qualities they have. First off, earth abundant precursors like C, H, O or N can be used to create organic compounds. Additionally, they do not use dangerous heavy metals that have a negative impact on the environment. In addition, compared to conventional inorganic material based batteries, organic redox active material based batteries have a huge potential to significantly boost energy storage capabilities. One fundamental challenge in developing novel energy storage devices based on organic electrode materials is to rapidly identify a subset of promising materials candidates that possess target Redox Potential (RP) computed at the desired fidelity from a large set of candidate materials.

Description

An exhaustive computational screening campaign is essentially impossible since there may be a sizable number of potential organic materials to be screened and because the estimation of RP at the necessary fidelity level may demand a significant amount of computer resources per molecule. Recent research has shown that Machine Learning (ML) models are useful for accurately predicting the links between structure and electrochemical properties. Based on ten predictive features the number of B/C/Li/O/H, aromatic rings, Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), HOMO-LUMO gap and electron affinity a fully connected Neural Network (fcNN) with two hidden layers accurately approximated the RP of molecules (EA). Despite their predictive effectiveness, these ML methods have not been consistently used in a goal driven computational screening programme. Instead, depending on the characteristics predicted by ML surrogates, their primary application has been to prioritise attractive materials for future study. Building a High Throughput Virtual Screening (HTVS) pipeline with various mathematical or surrogate models of varying fidelity and processing cost is one practical goal driven method for the efficient identification of viable candidates. These HTVS pipelines typically employ computationally efficient models in the early stages to effectively weed out samples that are unlikely to have the desired attribute. The remaining samples are moved on to the next stage for additional analysis using more accurate models, which likewise cost more to compute. The highest fidelity model is used to evaluate the molecules that continue to the penultimate stage for final validation. The key to

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an HTVS pipeline is to effectively distribute computing resources across several stages to maximize Return on Computing Investment (ROCI). HTVS pipelines have been extensively employed in a variety of domains, including biology, materials science, due to their capacity to quickly screen a huge pool of candidates. In the past, operational tactics for these HTVS pipelines have relied on expert intuition, which frequently leads to acceptable but subpar screening performance. To overcome this issue, a mathematical optimisation approach that optimizes the screening policy for throughput and computing effectiveness has recently been put forth. In order to maximise throughput and accuracy while minimising the demand on computational resources, the screening threshold values are jointly optimised based on an estimation of the joint score distribution that takes into account the relationship between the predictive scores computed at different stages. It was demonstrated that the optimised screening strategy efficiently accomplishes the screening campaign's goal while significantly increasing the HTVS pipeline's computing efficiency. This study assumes that the HTVS pipeline is already given and just the screening policy needs to be developed, which eliminates the need for and reliance on heuristic and poor screening rules. However, how should one build the HTVS pipeline if one can only find a high fidelity property prediction model that is computationally expensive and does not yet exist?. In other words, how should one construct lower fidelity surrogate models to be placed earlier in the HTVS pipeline, assuming that the supplied high fidelity model will be placed at the end of the pipeline, such that overall efficiency can be improved without degrading screening accuracy. The issue with the construction of the HTVS pipeline is still unresolved.

Conclusion

In this study, we propose a computational framework for addressing this challenge through the effective design and optimal operation of a High Throughput Virtual Screening (HTVS) pipeline that enables rapid screening of organic materials that satisfy the desired criteria. Starting from a high fidelity model for estimating the Redox Potential (RP) of a given material, we show how a set of surrogate models with different accuracy and complexity may be designed to construct a highly accurate and efficient HTVS pipeline. We demonstrate that the proposed HTVS pipeline construction and operation strategies substantially enhance the overall screening throughput.