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Application of Computational Alchemy to screen alloys of alumina (Al2O3) as a catalyst support

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Descriptors derived from density functional theory (DFT) calculations have been the standard when it comes to screening any alloy configuration space. However, deriving descriptors using DFT comes with high computational costs since any alloy configuration space is expansive. DFT derived descriptors have been used for scaling relationships (SR), quantitative structure property relationships (QSPR) and of late artificial intelligence/machine learning (AI/ML) in screening for alloys and catalysts. However, SR and QSPR still require lots of DFT calculations and AI/ML need lots of training data. Catalyst support have not been intensively investigated. Much of the focus has been on the catalyst. However, alumina (Al2O3) has been the most dominant support in use. Computational alchemy can be used to approximate a descriptor on a large number of random/hypothetical alloy configurations with low computational cost. This is because it only requires a single set of reference DFT calculations. Transition metal doped Al2O3 has been reported to possess excellent attributes, such as the ability to promote surface diffusion and prevent clustering/sintering by suppressing grain growth. In this study, using the binding energy as a descriptor, we screen for random/hypothetical alloys of the catalyst support Al2O3 using computational alchemy. We explore in this study, some of the limitations of challenges of this approach in screening for a broad range of alloys. Pt is introduced at different locations within the alloy matrix to make Al2O3 a conductor and suitable for computational alchemy. Like previous studies, on metal alloys, computational alchemy predicts adsorbate BEs in close agreement with those obtained using DFT calculations. This study provides insights on how computational alchemy can be useful in materials' predictions at low computational costs.

Student?

No

Supervisor name

Supervisor email

Primary authors: Dr OUMA, Cecil (HySA - Infrastracturte); Prof. BESSARABOV, Dmitri (HySA Infrastructure)

Presenter: Dr OUMA, Cecil (HySA - Infrastracturte)

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