Beyond d-band center to identify the catalyst for oxygen evolution reaction: DFT combined with interpretable machine learning

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Descriptors obtained through computational studies play important role in designing a catalyst for several catalytic reactions. A good descriptor can explain the catalytic activity and used to design newmaterials with selectivity. The d-band center is a well-known descriptor used for various reactions [1], however it fails to give significant correlation where the electronic environment is slightly for a same metal.
Using Density Functional Theory (DFT), single atom catalysts embedded on two types of graphene nanoribbons for pristine and doped cases are used to check the oxygen evolution reaction activity. From these systems, possible d-band and p-band based descriptors were individually tested and proved no correlation with OER activity [2]. The approach of using multi-descriptor instead of single descriptor is proposed to address the peculiar descriptor problem and can be extended to other electrocatalytic reactions. The d-band frontier and the d-band occupancy scaled by width corrected band center together correlates with OER activity for same metal site under varying electronic environment. 432 active sites tested for OER activity using DFT and 105 possible descriptors are individually assessed for activity correlation and optimized using PCA and 8 machine learning algorithms.

Also I will discuss about the Pipeline we are developing named as “Padarth Khoj” focused on finding catalysts and battery materials.

Reference:

1. Hammer, B.; Norskov, J. K. Why Gold Is the Noblest of All the Metals. Nature. 376, 1995, 238.
2. E. S. Erakulan, Sourav Ghosh, Ranjit Thapa, Site Specific Descriptor for Oxygen Evolution Reaction Activity on Single Atom Catalysts Using QM/ML, Journal of Materials Chemistry A, 12, 2024, 19176.