S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Condensed Matter Physics and Material Sciences

08th December'2021 4.00PM ONLINE

SPEAKER

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TITLE OF THE TALK

Energy and Electronic Descriptors of Carbon-based Catalyst Towards OER/ORR using Quantum Mechanics/Machine Learning Approach

ABSTRACT

Oxygen evolution reaction (OER) is a key aspect of energy conversion and storage technologies. The optimal electrocatalyst can speed up the sluggish kinetics of OER. The oxygen reduction reaction (ORR) is an important reaction that takes place in the cathode of a fuel cell, wherein molecular oxygen is reduced to water. It is important to understand the energy parameter which defines the activity. Recently, descriptor-based approach becomes efficient to search and design the correct catalyst for various reactions. The task is mammoth to find the best carbon catalyst in large material space but can be done through identification of correct features and subsequently using of machine learning tools. Using QM/ML approach, we proposed π–electronic descriptors and developed predictive models using simple fits, multiple linear regression and random forest regression to identify the best active site. As model structure we have consider heteroatom (S, P, SO2, PO2) edge-doped graphene nanoribbons. In DFT analysis, activity towards OER of 112 sites of the 14 structures is considered. Further 26 models, i.e. (4-, 5-, …to 20-) AGNR and (4-, 6-, …to 20-) ZGNR is taken to understand the effect of nanoribbon width. Further to find the catalyst for ORR we estimated the site-specific performance of 250 various active sites. With the help of the SVR model and nanoribbon width relations, then we predicted the ORR performance of nearly 2500 sites and listed a few efficient active sites of edge-doped graphene nanoribbons. We have shown that the QM/ML approach is more efficient towards the searching of highly active catalysts for OER/ORR, through reducing the computational cost and improving the prediction capability.

References
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HOST FACULTY

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