

Webinar

Understanding the Structure - Catalytic and Electron Transport Property Correlations of Graphitic Nanostructures and Platinum

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Nanomaterials are bringing in a new era of technology, as new materials with unique properties are being discovered. A deeper understanding of the problems of existing materials and hints to make new functional materials can only be gathered by understanding the structure-property relationship between the nanoparticle and its relevant use. In this scenario, we attempt to understand the catalytic properties (primarily hydrogen evolution) and electronic transport properties, using doped-graphene based structures and functionalized carbon nanotubes. Dynamics of reduction, nitrogen doping and nature of B/N doped species are studied for graphene oxide. The overall dynamics, bond formation and charging (due to external potential) have been simulated for an electrochemical understanding of water/ion dynamics on platinum. Lastly, the role of chemical linking of carbon nanostructures is studied, for the overall catalytic effect, and to understand the electronic nature of small molecule linkages in these systems. In all these cases, we observe that minor chemical changes can impart major functional changes.

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