

## Ab-Initio Computational Studies of Doped Graphene Catalysts in Fuel Cell Application

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Low temperature fuel cells with noble metal-based catalysts are one of the promising green technologies. They are faced with several challenges, however largely from catalyst materials such as high materials costs, poor electrochemical durability and low activity. As such, it is strongly demanded to develop inexpensive but efficient and stable metal-free catalysts.

This presentation show that graphene materials doped by N, B and P elements are promising to replace Pt catalysts in low temperature operating fuel cell applications. Using first-principles density functional theory (DFT) computations an atomic-level structural predictions are accomplished for the elemental doped as well as co-doped graphene materials in which catalytic activities are analyzed by calculating thermodynamic free energy diagrams and thus, identifying the most viable ORR mechanisms.

Our results indicate that doping a graphene with heteroatom causes significant charge redistribution around the dopant such that a positively charged site acts as O<sub>2</sub> adsorption site. Furthermore, two-electron reaction involving hydrogen peroxide was not preferred on N, B, and P-doped graphene but on pristine graphene.