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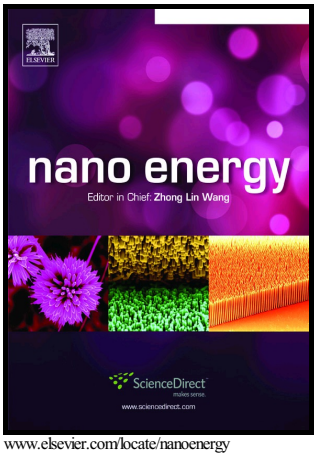

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Catalytic Mechanism and Design Principles for Heteroatom-Doped Graphene Catalysts in Dye-Sensitized Solar Cells

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ABSTRACT

Doped carbon nanomaterials are promising candidates to replace expensive Pt counter electrode for catalyzing triiodide reduction reaction (IRR) in dye-sensitized solar cells (DSSCs), but trial-and-error approaches have been used to develop better catalysts. Here, design principles are developed for p-block heteroatom-doped graphene as efficient IRR catalysts through density functional theory (DFT) calculations. Descriptors relating intrinsic properties of dopant elements are identified to establish a quantitative relationship that correlates the doped structures to catalytic activities. Moreover, a quantitative relationship is also established between the catalytic performance and the extrinsic factors such as the number of exposed active sites for a particular mass loading. It is predicted that dopants have their better performance than Pt, and that graphene hetero-edges facilitate catalytic activities. These predictions are consistent with experimental results. The proposed design principles enable us to rationally design and search for highly active catalysts based on earth-abundant, cost-effective materials.

Graphical abstract