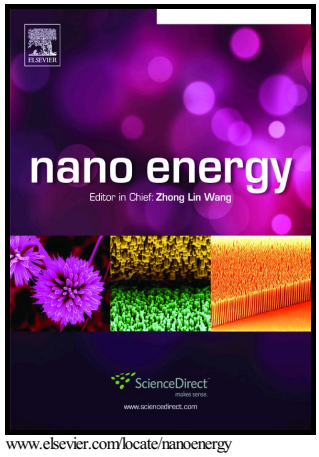

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Linking Structure to Function: The Search for Active Sites in Non-Platinum Group Metal Oxygen Reduction Reaction Catalysts

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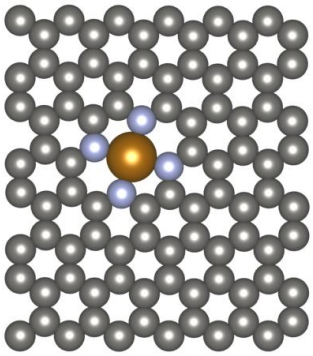
Abstract

Atomic-scale structures of oxygen reduction reaction (ORR) active sites in non-platinum group metal (non-PGM) catalysts, made from pyrolysis of carbon, nitrogen, and transition-metal (TM) precursors have been the subject of continuing discussion in the fuel cell electrocatalysis research community. Quantum chemical modeling is one path forward for understanding of these materials and how they catalyze the ORR. We here demonstrate through literature examples of how such modeling can be used to better understand non-PGM ORR active site relative stability and activity and how such efforts can also aid in the interpretation of experimental signatures produced by these materials.

TOC Figure:



Keywords: non-PGM catalysts; oxygen reduction reaction; ORR; DFT modeling; fuel cells

Background

The use of non-platinum group metal (non-PGM) catalysts for the oxygen reduction reaction (ORR) that occurs at the cathode of proton exchange fuel cells (PEFCs) is