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Two-dimensional iron-porphyrin sheet as a promising catalyst for oxygen reduction reaction: a computational study

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Abstract

The development of non-platinum (Pt) oxygen reduction reaction (ORR) catalysts with high activity and low cost is of great importance for large-scale commercialization of fuel cells. By means of density functional theory (DFT) computations, we theoretically identified that two-dimensional (2D) iron-porphyrin (Fe-Pp) sheet, in which the active Fe sites are distributed regularly and separately, is an appealing candidate. The pristine Fe-Pp sheet exhibits considerably high catalytic activity and four-electron selectivity for ORR. Especially, the adsorption of ORR intermediates on Fe-Pp sheet can be significantly weakened by the addition of axial cyanogens (CN) ligand, resulting in pronouncedly enhanced ORR activity. More interestingly, the d band center of CN attached Fe-Pp