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Computational Modeling of Nano Diode-like Heterostructures and Their Catalytic Performance for Oxygen Reduction Reaction[1] TAEGYUN KIM, HAIYING HE, STAN ZYGMUNT, Valparaiso Univ — Catalysts for the oxygen reduction reaction (ORR) are at the heart and remain a great challenge of electrochemical processes such as fuel cells and metal-air batteries. We have constructed diode-like heterostructure as potential ORR catalysts using four atom metal clusters (electron-poor) anchored on a graphene sheet (electron-rich). We have considered eight transition and noble metals including Fe, Co, Ni, Cu, Pd, Ag, Pt, Au. The charge transfer from the metal cluster to the graphene is well correlated with their electronegativity. As an initial test of the catalytic behavior of these heterostructures, we have calculated the oxygen adsorption. Fe, Co, Ni, Cu, Pt, and Pd metallic clusters with graphene all favor O_2 dissociative chemical adsorption, suggesting a preference of the dissociative mechanism for ORR. The implication of the calculated O binding energy to oxygen reduction activity will also be discussed.

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Taegyun Kim
Valparaiso Univ

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