Carbon-Supported Core-shell Nanoparticles as Oxygen Reduction Electrocatalysts and Their Enhanced Activity and Stability

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Core-shell catalysts for polymer electrolyte membrane fuel cells have the benefits of a high utilization of catalyst and the modification of its electronic structures toward enhancement of the activities. In this study, we computationally screened the potential core@shell combination and devised a facile synthesis route for the proposed structures. To determine the best core@shell combinations for ORR, we performed density functional theory (DFT) calculations using two descriptors. The first descriptor is the oxygen adsorption energy (OAE) on the Pt shell to measure the reactivity. The other descriptor is the vacancy formation energy (VFE) of Pt in the Pt shell to measure stability proposed in this study.