Theoretical analysis on active site and reaction mechanism in N and B doped graphene as cathode catalyst of fuel cell

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Abstract: Recent studies suggest that the carbon-alloy catalyst with doped N and B may be a powerful candidate for cathode catalyst of fuel cell [1-3]. We aim to clarify the microscopic mechanisms of the enhancement in the catalytic activity caused by N and B doping using a simple graphene cluster model [4]. Our analysis is based on the density-functional electronic structure calculations. We also simulate the processes of oxygen molecule adsorption to carbon-alloy catalyst and subsequent oxygen reduction reaction using the first-principles molecular dynamics [5,6].

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