Development of new electro-catalyst through combining with experimental and ab-initio computational calculation in electrochemical energy conversion systems

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Development of highly active electrocatalysts that are cost competitive takes the center stage in research fields for next-generation electrochemical energy conversion and storage systems like fuel cell and metal-air battery. Regarding the systems for commercialization, there are many challengeable issues, which should overcome sluggish kinetics and stability on the electro-catalyst for the aimed reactions such as oxygen reduction reaction (ORR) or oxygen evolution reaction (OER) occurred in the high over-potential and harsh condition. By applying first principles calculations and state of the art experimental measurements to well-defined model systems of metals, metal oxides and Pt nanoparticles with heteroatom-doped graphene for ORR/OER, we unveil the fundamental mechanisms controlling the catalytic properties and structural integrity of targeted catalysts. The key factors governing the catalytic performance were provided through the electrochemical and physicochemical analyses, calculating the dissolution potential, cohesive energy, free energy change for each reaction.