J Phys Chem Biophys 2017, 7:2(Suppl)
DOI: 10.4172/2161-0398-C1-020

First principles design of an active electrocatalyst toward oxygen involved reactions through self-assembled fullerenes from graphene

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Using first principles-based calculations we design a self-assembled fullerene (N-fullerene) from N-doped graphene fragments, which is active for oxygen reduction (ORR) and evolution reaction (OER), applying to energy conversion and storage devices such as fuel cells, metal-air batteries systems. We screen the best N-fullerene catalyst at 10 at.% doping level of nitrogen not at previously known 5 or 20 at.% for graphenes. We identify that compressive surface strain induced by the doped nitrogen plays a key role in the fine-tuning of the catalytic activity.

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Anion conductors: New materials for chloride and fluoride ion batteries

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Anions, from a chemical point of view are at the opposite end of the standard reduction potential series from lithium, and therefore, show interesting possible applications in battery systems.The general working principle of such an anion battery is based on the reduction of the cathodic material and the oxidation of the anodic material via anion transport through the electrolyte. An example is given here (Figure 1) with iron salt as cathode and metallic magnesium as anode. But for obtaining an anion battery a good ionic conduction is required throughout all parts of the cell such as cathode, electrolyte and anode to assure the migration of chloride ions or fluoride ions. Our work focuses on understanding anion migration and to develop new materials with good halogenide conduction. In this talk, the latest advances and challenges in room-temperature fluoride ion batteries and chloride ion batteries will be presented.

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