Multiscale Computational Design of Highly Functional Carbon for Renewable Energy Materials

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Using first-principles density functional theory calculations and ab-initio molecular dynamic simulatons we propose design principles for key materials in energy systems to improve energy and power efficiency. It is shown that functional carbons can play a role to substantially improving the activity and durability of catalysts for oxygen reduction reaction (ORR) in Proton electrolyte membrane (PEM) fuel cells and Li-air batteries ion batteries. Free energy diagram and Pourbai diagram are illustrated as an important tool estimating the performance of the carbon materials. It is presented that smart design of inorganic nanocatalyst particles can be further optimized by thin doped carbon or graphite shells, which are self-assembled, to overcome the conventional limits of Pt-based catalysts. Finally, we show that the approach is developed into a universal computational framework to design any material as required for the system.

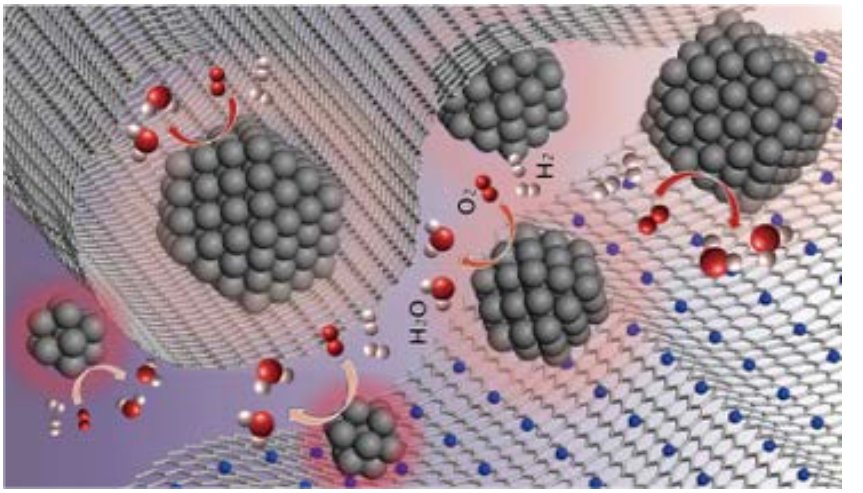

Figure 1: Computationally designed Pt/C catalyst for ORR in PEM fuel cell. [1]

References
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