Computational model of the catalytic activity of monolayer amorphous carbon in hydrogen evolution reaction

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Abstract

We present a computational study on monolayer amorphous carbon (MAC), a topologically disordered sp^2-hybridized carbon film, and promising alternative to expensive noble metal electrocatalysts [1]. Our findings indicate that out-of-plane buckling and an enriched electronic density of states near the Fermi level, both introduced by the high density of non-hexagonal rings, give rise to MACs enhanced catalytic activity towards hydrogen evolution reaction (HER). Using density functional theory (DFT), a broad distribution of hydrogen adsorption free energy values (ΔG_H) is further revealed, containing a significant number of active sites ($\Delta G_H = 0$) evenly scattered across the basal plane—setting MAC apart from other emergent 2D catalysts with activity confined to the edges [2][3]. The broadness of the distribution moreover suggests that, unlike conventional single-active-centre catalysts (e.g., Pt), MAC's catalytic activity may remain stable under varying conditions—such as changes in proton concentration or other environmental factors.

References

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Figures

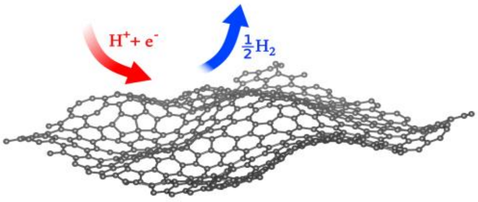

Figure 1: Schematic illustration of MAC as a HER catalyst.