

CURVATURE EFFECTS ON THE REACTIVITY OF NANOMATERIALS

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Different forms of carbon such as graphene, nanoribbons, and nanotubes exhibit different curvature. It has been found that curvature on graphene layers can affect some of their properties. A few studies have focused on the reactivity, but mainly in surface regions. The effect of curvature is more uncertain at the edges of nanocarbon materials. In this study we compare thermodynamics and kinetics of adsorption and desorption reactions path of hydrogen and oxygen on carbon nanomaterials, considering both the edges and the surfaces. Size effects of the graphene layers are also evaluated. It is found that curvature has an important effect on the stability of the adsorbed states.