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Morphological, electronic, and catalytic properties of Pt nanoclusters on defective graphene IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — The synthesis of well dispersed, size-controlled Pt nanoclusters on carbon supports is highly desirable since such clusters have been shown to possess enhanced catalytic activity and selectivity in a variety of chemical reactions. However, these nanoclusters interact rather weakly with defect-free carbon supports and can coarsen over time leading to loss of surface area and thence catalytic activity. Defects in carbon supports play an important role in enhancing Pt-carbon bonding, thereby reducing the propensity for cluster coalescence. Using a combination of density functional theory and empirical potential simulations, we examine the interaction of Pt nanoclusters with point defects in graphene. We focus on the role of the support defects in controlling the morphology, electronic structure, and CO-tolerance of Pt nanoparticles. Our results suggest possible avenues for controlling the dispersion and activity of Pt nanoclusters on carbon supports via defect engineering.

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