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Catalytic properties of Pt nanoclusters on defective graphene IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — Metal nanoparticles on carbon supports hold promise as electrocatalysts in direct methanol fuel cells, proton-exchange membrane fuel cells, and hydrogen fuel cells. Pt nanoclusters on carbon supports have been shown to possess superior catalytic activity and increased selectivity in a variety of electrochemical reactions as compared to bulk Pt electrodes; however, the underlying mechanisms remain poorly understood. We examine the interaction of Pt nanoclusters with point defects in graphene using first-principles density functional theory. The presence of defects in graphene supports enhances the Pt-carbon bonding, which suppresses cluster sintering thus allowing for sustained catalytic performance. Furthermore, stronger binding of clusters at defects is found to increase the tolerance of bound Pt nanoparticles towards CO poisoning. Finally, we examine the role of defective graphene supports on the activity of the cluster for the CO oxidation reaction and obtain estimates for CO-oxidation kinetics. Our results suggest possible avenues for controlling the dispersion and catalytic activity of Pt nanoclusters on carbon supports via defect engineering.

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