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Catalytic Properties of Graphene-Supported Pt13 Nanoclusters IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — Graphene is of considerable interest as a support material for fuel cell electrodes due to its high surface area, high mechanical strength and exceptional electrical conductivity. Here, using density functional theory calculations we investigate the electronic and catalytic properties of Pt_{13} clusters supported on pristine and defective graphene. We show that defects in the graphene support significantly stabilize Pt clusters against sintering. Strong cluster-substrate interactions are also found to substantially shift the d band centers of the Pt clusters. Specifically, we investigate the adsorption of CO and O on Pt clusters bound at defects in graphene and show that such defect-supported clusters adsorb CO and O more weakly than clusters supported on pristine graphene or entirely unsupported clusters. We examine the kinetics of the CO oxidation reaction and demonstrate that graphene-supported Pt_{13} nanoclusters–despite the low coordination of surface atoms–possess comparable catalytic activity with macroscopic Pt(111) surfaces and, in general, superior catalytic activity compared to unsupported clusters. Our results suggest possible avenues for controlling the dispersion and catalytic activity of Pt nanoclusters on graphene supports via defect engineering.

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