

Abstract Submitted
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Carbon Nanotube – Supported Metal Nanoparticles: Properties of Novel Heterogeneous Catalysts Predicted by Molecular Simulations

ALBERTO STRIOLO, BRIAN MORROW, University of Oklahoma — We conducted all-atom molecular dynamics simulations for Pt nanoparticles composed of 150-500 atoms on either graphite or bundles of CNTs. The CNTs considered are (4,4), (10,10), and alternating (10,10) and (4,4) CNTs. The diameter of the simulated Pt nanoparticle is comparable to those typically employed experimentally. Our results suggest that the substrate strongly influences the morphology of the Pt nanoparticles, in particular the number of Pt atoms with low-coordination number (characterized by higher chemical reactivity). Results for diffusion coefficients of the Pt nanoparticles on CNTs are one order of magnitude lower than those on graphite, suggesting that Pt sintering is less likely on CNTs than on graphite. At low temperature the Pt nanoparticle resides within the trench formed by two adjacent CNTs, but at high temperature it is located on top of one CNT. If supported by experimental data, the results presented here could lead to the production of catalysts that are stable at very large operating temperature.

Alberto Striolo
University of Oklahoma

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