

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Properties of Pt_{37} and $\text{Pt}_6\text{Ru}_{31}$ Clusters on Carbon: comparison of theory and experiment¹ LIN-LIN WANG, DUANE D. JOHNSON, Department of Materials Science and Engineering, UIUC — Using DFT calculations, we analyze the structures of self-organizing nanoparticles formed by Pt and Ru-Pt on a carbon support and clarify complex behaviors noted in earlier experimental studies. With clusters deposited via metallo-organic Pt or PtRu5 complexes and annealed at 670 K in hydrogen atmosphere, the Pt and Pt-Ru based clusters were observed to form fcc(111)-stacked cuboctahedral geometry and essentially bulk-like metal-metal bond lengths, even for the 10-40 atom nanoparticles for which the average coordination number is much smaller than that in the bulk, and that Pt in bimetallic clusters segregates to the ambient surface. We explain these observations and characterize the cluster structures with graphite as a model for the support. Our study reveals the origin of the observed bulk-like metal-metal bond lengths and bond-length disorder, and demonstrates the profound consequences that result from the cluster/support interactions and hydrogen passivation on their structural and electronic properties.

¹DOE Grants DE-FG02-91ER45439 and DE-FG02-03ER15476

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Date submitted: 30 Nov 2005

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