

## Properties of Supported Catalytic Nanoparticles – Theory and Experiment: Dependency on Size, Support, and Adsorbates

**Duane D. Johnson\***

Division of Materials Science and Engineering, Ames Laboratory/US DoE Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011

From an orchestrated study using *ab-initio* simulations and advanced characterization methods (i.e., HR-TEM, environmental-TEM, and EXAFS), we highlight results for supported nanoparticle (NP) involving key *structure-property* relations that are critical for *structure-property-function-design* paradigm in catalysis science. Yet to be fully understood for supported NPs are – structure vs. size, cluster vs. ensemble, and ergodic vs. non-ergodic behavior (found when a support contains surface defects, e.g., O vacancies). While bulk amorphous Pt is unstable, theory predicts and experiment confirms (with observations of over 3000 NPs) that there is an *amorphous-to-crystalline* transition for supported NPs depending on cluster size, support and adsorbates. Existence of amorphous NPs is a manifestation of their mesoscopic nature, a behavior in distinct contrast to unsupported NPs. We will highlight structural properties of Pt NPs on C or  $\gamma\text{-Al}_2\text{O}_3$  in an inert and reactive atmosphere, with emphasis on theoretical results and connection to experimental results – including care needed in simulations. We show that a statistical description is necessary to describe the structural behavior, emphasizing the need for complementary characterization methods. We also discuss the *two key factors that control the core-shell behavior of binary NPs*, which also works for bulk alloy surface – for rapid prototyping.

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