EMSL Research and Capability Development Proposals

Molecular-scale Visualization of Ligand Conformation on Functionalized Nanoparticles: A Combination of Experimental and Theoretical Studies

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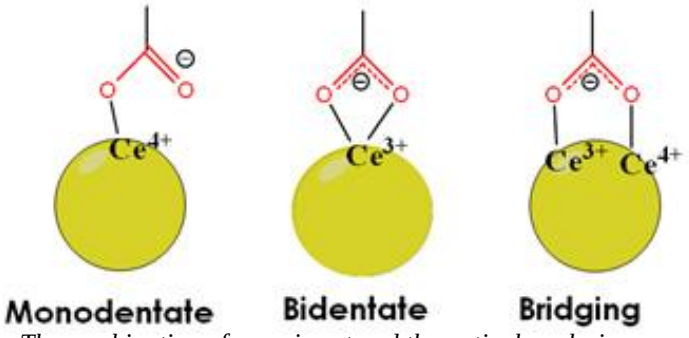
The goal of this project is to develop capabilities that will advance the fundamental understanding of the interaction between nanoparticle surfaces and organic ligand molecules as applicable to dye-sensitized solar cells, contamination remediation in groundwater, and drug delivery in biological systems. This would be accomplished by using cerium oxide (CeO_2) nanoparticles and organic ligands with carboxylate and phosphonate functional groups; applying existing and newly developed tools at EMSL to characterize the nanoparticle–ligand interactions; and measuring the impact of the derivatives on the organic ligands, the variation of the surface potential of the nanoparticles, and their particle sizes. The results on these systems will provide information about the structural and electronic aspects at the molecular level, the chemical state of elements in the nanoparticle and organic coating, the number of ligand molecules on the particle surface, and their orientation and nature of packing. Mainly, non-linear optical methods**,** sum frequency generation-vibrational spectroscopy (SFG-VS), and the second harmonic generation (SHG) will be used to characterize the functional groups and their conformation on the nanoparticle surfaces (i.e., the bonding sites, bond strength, and bond directions of ligand molecules on ceria nanoparticles). However, X-ray photoelectron spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, and electron microscopy also will be used to determine characterization. First-principle calculations will provide critical insights into the surface structure, conformation of binding ligands, and chemical nature of bonding interactions. The combined and complementary data sets from theoretical studies and experimental efforts will visualize and elucidate the often complicated nature of CeO_2 nanoparticle–ligand systems and extend the understanding to other relevant systems in the future,



The combination of experiment and theoretical analysis will be used to predict the bonding characteristics of the ligands on cerium oxide nanoparticles.

providing essential knowledge to teams poised to address the issues of fundamental and applied interest in nanoparticle research.

Products and Output

New Capability for EMSL Users

This is an evolving area of research in EMSL that combines theory and experiment aimed at potential future program development.

Presentations

Karakoti A.S., S. Kuchibhatla, G. Orr, H. Wang, D.R. Baer, S. Seal, and S. Thevuthasan. 2010. "Functionalized Ceria Nanoparticles–Influence of Coating Thickness and Density on Their Reactivity." submitted to *AVS 57th International Symposium & Exhibition*, October 17-22, 2010, Albuquerque, New Mexico.