

UC San Diego

JACOBS SCHOOL OF ENGINEERING
Aiiso Yufeng Li Family Department of
Chemical and Nano Engineering

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DEPARTMENT SEMINAR

Wednesday, November 20th, 2024

11:00 AM - 12:00 PM

SME 248

Dr. Ping Yang, PhD

“Structure, Stability, and Chemistry of Actinide Nanoparticles”

Deputy Director, G.T. Seaborg Institute for Transactinium
Science

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Abstract: Nanoscale materials bearing heavy elements have a wide range of applications from the nuclear fuel cycle to environment and health. Nanocrystals (NCs) with size and shape dependent properties are a thriving research field and remarkable progress has been made in the controlled synthesis and characterization of NCs composed of stable elements in the past three decades. In this context, interfacial chemistry of nano-sized materials is critical for controlling the morphology that drives their unique associated chemical and physical properties. The understanding of NCs containing f-elements is comparatively limited due to difficulties in handling them both experimentally and theoretically. In this talk, I will share some recent progress in understanding the interplay between surface energy, surfactant ligands, and the chemistry in determining the morphology of 5f-element nanoparticles. Quantum simulations provide a molecular-level picture of the relevant driving forces and dynamic properties. To push for larger lengthscale and longer timescale, we recently developed the density functional theory tight-binding (DFTB) parameters for actinide systems, that enabled the microsecond quantum MD simulations of actinide nanoparticle systems.

[1] G Wang, ER Batista, P Yang. *Phys Chem Chem Phys* 2018, 20, 17563

[2] G Wang, ER Batista, P Yang, *J. Phys Chem C*, 2019, 123, 30245

[3] NF Aguirre, J Jung, P Yang, *Phys Chem Chem Phys* 2020, 22, 18614

[4] D G Gonzalez, G Wang, ER Batista, P Yang, *Inorg Chem* 2023, 62,14852

[5] C Liu, N Aguirre, M Cawkwell, ER Batista, P Yang, *J Chem Theory Comput*, 2024, 20, 5923

[6] D Burrill, C Liu, MG Taylor, M Cawkwell, N Lubbers, D Perez, ER Batista, P Yang, 2024,

10.26434/chemrxiv-2024-0n3q0

Bio: Ping Yang serves as the Deputy Director of the G.T. Seaborg Institute for Transactinium Science and a Staff Scientist in the “Physics and Chemistry of Materials” group of the Theoretical Division at Los Alamos National Laboratory (LANL). Yang’s research aims to elucidate the fundamental electronic structure and reactivity of actinides complexes, nanoparticles, and surfaces. She holds a keen interest in leveraging high-performance computing frameworks and data science to develop new computational techniques for simulating complex actinide systems over long timescales, and to accelerate f-element separation.

Seminar Host: Wanlu Li