



Materials Science and
Engineering

MSE COLLOQUIUM SPEAKER

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Zoom Link: <https://ucr.zoom.us/j/95770338533?pwd=anQ4YjNTNzNnQ3M3U2EvOFgrT2E5dz09>

Computational Methods for Atomic-scale Investigation of Materials

Interactions between heterogeneous systems are challenging to model with high fidelity at the atomic and electronic structure scales. Computational methods at the level of first-principles density functional theory (DFT) calculations and classical reactive potentials are used to quantify structure-property relationships in heterogeneous systems in a way that is highly complementary to experimental data. This presentation will focus on the investigation of the properties of two-dimensional material which have properties that strongly depend on composition, defects, and surface structure. Here, DFT methods are used to investigate the structure-property dependence of two-dimensional MXenes and carbon-doped metal dichalcogenides. The computational predictions are compared to experimental data to advance design of two-dimensional materials. Recent developments of classical, third-generation charge optimized many-body (COMB3) potentials and their utilization in atomistic simulations to investigate the oxidation and dissolution of metal catalysts in water is also discussed.



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Dr. Sinnott received her B.S. in chemistry from the University of Texas at Austin and her Ph.D. in physical chemistry from Iowa State University. She was a National Research Council Postdoctoral Associate at the Naval Research Laboratory and was on the faculty at the University of Kentucky prior to moving to the University of Florida in 2000. In 2015 Susan joined The Pennsylvania State University as Professor and Department Head of Materials Science and Engineering. Dr. Sinnott is the author of 290+ technical publications, including 270+ refereed journal publications and is a Fellow of the Materials Research Society, American Physical Society, American Ceramic Society, American Vacuum Society, and of the American Association for the Advancement of Science. She is a past President of the American Vacuum Society and is the Editor-in-Chief of Computational Materials Science.