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MATERIALS SCIENCE & ENGINEERING DISTINGUISHED SEMINAR SERIES

Susan B. Sinnott, Ph.D.

Professor and Department Head
Materials Science and Engineering
Pennsylvania State University

Friday
February 21, 2020

11:00AM — 12:00PM

Research 1

Room 101

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Classical Atomic-scale Methods in Material Design and Discovery

A driving force for research is the discovery and design of new materials to improve existing technologies or enable new applications. Classical atomic-scale methods are now widely applied in pursuit of this objective. This presentation will review the evolution of some common material modeling methods and their integration with cutting-edge experimental techniques. Illustrative applications will be discussed within the context of water-metal interfaces and carbide-derived carbon materials.

Biography: Susan B. 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 joining the University of Florida in 2000. In 2015 Susan joined the Pennsylvania State University as Professor and Department Head of Materials Science and Engineering with an affiliate appointment in the Department of Chemistry. Research in the Sinnott Group is focused on the application of computational methods at the electronic-structure and atomic scales to examine a variety of materials and processes. These include the design of new materials and the investigation of the influence of grain boundaries, point defects, dopants, and heterogeneous interfaces on material properties. A major area of emphasis is the development of inventive methods to enable the modeling of new material systems at the atomic level. Susan is the author of 275+ technical publications, including 260 refereed journal publications. She 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. Susan is a past President of the American Vacuum Society and is the Editor-in-Chief of *Computational Materials Science*.