



**Wednesday**  
**October 25, 2023**  
**3:00 pm**  
**Room 1010 Dow**

# Prof. David B. Graves

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## Modeling and Simulation of Plasma-Surface Interactions in Nanofabrication

Plasma-enhanced atomic layer deposition (ALD) and etching (ALE) in principle offer an unprecedented opportunity to control surface composition and structure in various thin film-based nanofabrication applications. By modulating process time, frequency, energy, and chemistry, it is possible to vastly increase the range of conditions and surface modification effects at surfaces. ALE/ALD can simplify the process by separating, for example, a chemical surface modification step from addition of energy through rare gas ion bombardment. It might be possible to design novel etch and/or deposition precursor molecules to take advantage of ALE/ALD modulation-oriented approaches. However, process modulation introduces the complexity of having the surface state change in time during the exposure. To understand and control these processes, atomic scale plasma-surface interaction simulations are essential. In this talk, I briefly review the use of molecular dynamics (MD) simulations in plasma-surface interactions and how they have been used to help understand conventional plasma etching and deposition. I then use our recent studies of PEALD to highlight both successes and limitations of the current state of the art when used for modulated atomic layer processes. The key issues of interatomic force fields for many new chemistries and materials; using MD to simulate an intrinsically multi-timescale process; and the need to couple well-diagnosed experiments with atomistic simulations are emphasized.

**About the Speaker:** David B. Graves joined the U. of California at Berkeley Dept. of Chemical Engineering in 1986 after receiving his PhD from the U. of Minnesota. He retired from UCB in May 2020 and joined the Princeton Plasma Physics Lab and Princeton University, Dept. of Chemical and Biological Engineering. He served as Associate Lab Director at PPPL from 2020-22 where he is now Faculty Research Scientist. His research interests are in plasma materials processing, biomedical and other applications of non-equilibrium, low temperature plasma phenomena. His group studies the physics, chemistry, and biology of chemically active low temperature plasmas. David Graves is a fellow of the American Vacuum Society (AVS), the International Plasma Chemistry Society and the Institute of Physics. He is the recipient of the Electrochemical Society Young Author Award, the NSF Presidential Young Investigator Award, the Tegal Plasma Thinker Award, and the Plasma Prize of the Plasma Science and Technology Division of the AVS. He was the Lam Research Distinguished Chair in Semiconductor Processing at UCB for 2011-16. He received the Allis Prize for the Study of Ionized Gases from the American Physical Society in 2014 and the 2017 International Symposium of Dry Processes Nishizawa Award. In 2022 he received the Plasma Materials Science Hall of Fame Prize from Nagoya University, Japan.