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**12:00 pm**  
**BRK 1001**

## **The NIST Interatomic Potentials Repository -- a resource for reproducibility in atomistic simulations**

### ***Abstract:***

Atomistic simulations, such as molecular dynamics, are becoming more widely used in a variety of areas, including industrial research and development. However, there are still barriers to the broad use of these methods, both on their own and as part of an Integrated Computational Materials Engineering (ICME) or multi-scale/hierarchical approach. In this talk, we will discuss some of these barriers and recent efforts to address them. In particular we will discuss efforts at NIST to provide tools and resources to make interatomic potentials more widely available and means to select from among the many options. We will also discuss how this fits into the Materials Genome Initiative and highlight major issues identified in the annual NIST "Atomistic Simulations for Industrial Needs" workshops that are designed to facilitate interactions between industrial and academic researchers.

### ***Speaker Bio:***

Dr. Becker received her Ph.D. in Materials Science and Engineering from Northwestern University in 2006, advised by Prof. Mark Asta. She completed a National Research Council NIST postdoctoral fellowship and was subsequently hired as a member of the NIST scientific research staff in 2009. The focus of her work is the development of methods and tools to facilitate the engineering use of molecular simulation, particularly through the effective use of interatomic potentials (force fields).