Abstract Submitted
for the GEC18 Meeting of
The American Physical Society

Bridging the scales of simulations for plasma material interaction LONGTAO HAN, Stony Brook University, IGOR KAGANOVICH, Princeton Plasma Physics Laboratory, PREDRAG KRSTIC, Stony Brook University — It is important to understand how plasma properties influence the surface processes of materials in different levels, which may explain the synthesis, phase change or damage of materials. This talk will give an overview on simulation approaches that are being used in the modeling of plasma material interaction. Density functional theory methods (molecular DFT, plane wave DFT), quantum classical molecular dynamics methods (e.g., DFTB, DC-DFTB), classical molecular dynamics (e.g., LAMMPS) and kinetic Monte Carlo methods will be covered with examples in recent studies.

Longtao Han
Stony Brook University

Date submitted: 18 Jun 2018 Electronic form version 1.4