Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Development of an improved molecular dynamics force field for surface-adsorption simulations of molybdenum disulfide GARY LEUTY, National Research Council/Air Force Research Lab, RAJIV BERRY, Air Force Research Laboratory, CHRISTOPHER MURATORE, University of Dayton, VIKAS VARSHNEY, Air Force Research Laboratory, HEATH TURNER, University of Alabama — Transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS_2) have garnered significant interest in recent years. With a layered structure similar to graphene, TMDs also have an intrinsic band gap. This band gap makes them an attractive alternative to graphene in many applications. MoS_2 in particular has received attention due to the placement and tenability of its band gap, via functionalization, mechanical manipulation or physisorption. The latter of these is of interest in biosensor devices. Such applications are dependent on understanding physisorption on the MoS_2 surface at the molecular level. This can be difficult experimentally but is possible via computer simulation techniques such as molecular dynamics (MD) simulations. MD simulations, however, require a force field accurate to the process modeled. Such a force field must correctly describe non-bonded interactions between substrate layers and between the surface and adsorbates. The force fields we are aware of have focused on intra-layer covalent bonding for structural and vibrational analysis. This work seeks to develop, through DFT and MD simulations with experimental characterization of surface adsorption, a more accurate parameterization for non-bonded interactions for MoS_2.

Gary Leuty
National Research Council/Air Force Research Lab

Date submitted: 06 Nov 2015 Electronic form version 1.4