Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Computational study of electronic and thermal properties of single-layer molybdenum disulphide folded nanostructure JIE PENG, PETER CHUNG, Univ of Maryland-College Park — Single-layer Molybdenum disulphide ($SLMoS_2$), a two-dimensional transition-metal dichalcogenide with a large band gap and high mobility, is considered to be a next generation material for transistors and optoelectronic devices. We present recent results on the electronic and thermal behavior of $SLMoS_2$ folded nanostructures. Through an approach that uses both molecular dynamics (MD) and density functional theory (DFT), we estimate the stable equilibrium structure of folded sheets as well as the related phonon and electronic band structures. The MD simulations are based on a Stillinger-Weber potential and the DFT simulations employ projector augmented wave (PAW) pseudopotentials using generalized gradient approximation (GGA) and local density approximation (LDA). The structure is examined as a function of folding orientation, layer number and system size. Mechanisms of the phonon transport and electronic band gap properties in such a mechanically distorted atomic-layer nanostructure will be discussed.

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Date submitted: 06 Nov 2015 Electronic form version 1.4