Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Effect of Interlayer Interaction on the Structural, Electronic, and Thermal Properties of Layered MS_2 (M=W, Mo) Structures SEOUNG-HUN KANG, SORA PARK, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using density functional theory (DFT) supplemented with van der Waals interaction, we investigate the effect of interlayer interaction on the structural, electroinic, and thermal properties of transition-metal disulfides MS_2, such as MoS_2 and WS_2. We calculate the relative stability of various layer-layer stacking configurations determined by considering relative positions and orientations between neighboring layers. We find that MS_2 layers may slide over each other with a small sliding barrier. We explore the effect of layer stacking on the electronic structure, and find an intriguing coupling effect. We also calculate their thermal properties including thermal expansion behavior especially along the direction normal to the plane. Such thermal expansion behavior is considered for our study of Li-intercalation into layered MS_2, which may become a fundamental understanding for future development of Li-ion battery. We evaluate thoroughly the diffusion paths and barriers in between layers and compare them with those on the surface. Interestingly we find that the diffusion barrier between layers is $\sim$100 meV smaller than that on a single layer, implying layered MS_2 may be a good candidate for Li-ion battery electrodes.

Young-Kyun Kwon
Department of Physics, Kyung Hee University

Date submitted: 11 Nov 2011 Electronic form version 1.4