Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Raman spectrum of MoS2/WS2 heterostructure from first-principles calculation of phonon electron coupling[1] JUN JIANG, XIAOGUANG ZHANG, Univ of Florida - Gainesville, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, GEORGIOS D. BARMPARIS, Crete Center for Quantum Complexity and Nanotechnology, Department of Physics, University of Crete, Heraklion 71003, Greece, YEVGENIY S. PUZYREV, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA
— We present a first-principles method to calculate Raman spectrum of MoS2/WS2 heterostructure due to electron excitation. The first step is to calculate the ground state phonon modes and the displacements of the atoms from the ground state to the excited states. In the next step, Inelastic multi-phonon relaxation for the excited electron is considered to produce the Raman spectrum quantitatively. The relative Raman intensity, peak width and shape are obtained directly from a sum over trillions of configurations of multiple phonon modes using a Monte Carlo scheme. Alternatively, we also calculate the overlap between the ground state phonon mode eigenvectors and the excited state atomic displacements, which provides a quick and qualitative description for the Raman shifting due to electron excitation.

[1]This work is supported by NSF grant 1508898.

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Date submitted: 05 Nov 2015 Electronic form version 1.4