Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles Raman spectra of MoS_2, WS_2 and their heterostructures[1] LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute — MoS_2 and WS_2 are graphene-like layered structures that are considered as alternative and complement to graphene. Raman spectroscopy is a very powerful tool to study them. Despite the extensive experimental Raman study on MoS_2 and WS_2, it remains unclear how Raman intensities and especially intensity ratio of Raman modes E_{2g} and A_{1g} depend on the thickness. To clarify such issues, we carried out density functional theory calculations for both MoS_2 and WS_2 to simulate their Raman spectra and reveal the intrinsic thickness dependence of Raman intensities and intensity ratio. More importantly, we quantitatively analyzed the laser polarization effect on the intensity ratio and revealed its high sensitivity to laser polarization, which could explain the large discrepancy between measured intensity ratios by different groups. We also studied *ab initio* Raman spectra of MoS_2/WS_2 heterostructures up to four layers in every possible combinations and stacking orders. Each configuration is found to possess a unique Raman spectrum in both frequency and intensity that can be explained by changes in dielectric screening and interlayer interactions. Our findings serve as guidelines for the experimental identification of heterostructure configurations.

[1]The authors are supported by New York State under NYSTAR contract C080117 and by the US Army Research Laboratory through the Multiscale Modeling of Electronic Materials Collaborative Research Alliance.

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Date submitted: 14 Nov 2013 Electronic form version 1.4