Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The nature of interactions in layered two-dimensional transition metal dichalcogenides - Anomalous frequency trends and surface effects[1]

XIN LUO, SU YING QUEK, National University of Singapore and Institute of High Performance Computing — MoS_2 is a prototypical layered dichalcogenide material, with interlayer interactions dominated by weak van der Waals (vdW) interactions. Recent Raman experiments reported an anomalous blue-shift of the E^1_{2g} mode with decreasing thickness, a trend that is not understood by simply relating frequencies to the restoring force in the system. Here, we combine experimental and theoretical studies to clarify and explain this trend.[1] We show that although interlayer interactions are weak in these materials, removing layers to form a surface in thin film MoS_2 can lead to larger Mo-S force constants at the surface ("surface effect"), which in turn accounts for the observed anomalous frequency trend. We predict the same anomalous trends for other modes in layered WSe_2, which are confirmed by experiments [2]. We find that most of the important interactions responsible for this "surface effect" occur within $\sim$ 1.5 Å of the equilibrium interlayer distance. Our results have significant implications on the nature of interactions in vdW layered transition metal dichalcogenides.

[1] PRB 88, 075320 (2013);
[2] PRB accepted (2013)

[1]We gratefully acknowledge funding from Singapore NRF, A*STAR, MOE and NTU.

Suchun Li
National University of Singapore and
Institute of High Performance Computing

Date submitted: 12 Nov 2013 Electronic form version 1.4