Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Size reduction in layered semiconducting compounds TIANSHU LI, GIULIA GALLI, Department of Chemistry, University of California, Davis — In the last decade numerous experiments have shown dramatic changes in the optical properties of bulk semiconductors as their size is decreased to nanoscale dimensions. Most investigations have focused on 3D compounds such as II-VI and group IV. A few experiments have also been conducted for layered semiconductors, such as transition-metal dichalcogenides, indicating changes in photoluminescence properties apparently comparable to those found in 3D systems. We present extensive electronic structure calculations of the structural and electronic properties of MoS_2 nanostructures showing no appreciable quantum confinement effects in single sheet nanoparticles, whose electronic structure is dominated by the surface and in particular edge states near the Fermi level. On the other hand, a strong dependence of the electronic structure is observed as a function of layer stacking and distance. We suggest that the observed photoluminescence variation as a function of size does not pertain to size reduction in single sheets but rather to the number of planes composing the nanoparticle. We also suggest a way to engineer metallic nanowires taking advantage of edge states in nanosheet composites.

Tianshu Li
Department of Chemistry, University of California, Davis

Date submitted: 22 Nov 2006 Electronic form version 1.4