Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Dynamical charge and structural strain in MoS2 and MnO nanoparticles[1] QI SUN, XIAOSHAN XU, JANICE MUSFELDT, University of Tennessee, RESHEF TENNE, Weizmann Institute of Science, ALLA ZAK, Weizman Science Park, SHEILA BAKER, ANDREW CHRISTIANSON, Oak Ridge National Laboratory — We measured the far infrared vibrational properties of bulk and nanoscale MoS_2 and MnO in order to investigate finite length scale effects and chemical bonding in these materials. From an analysis of frequencies, oscillator strengths, and the high frequency dielectric constants, we extract Born and local effective charges for both materials. In the intralayer direction of MoS_2, we find that the Born effective charge of the nanoparticles is decreased significantly compared to the layered bulk, a result that we attribute to structural strain (and resulting change in polarizability). Preliminary results on the 7 nm MnO nanoparticles suggest that structural strain impacts both polarizability and depolarization field.

[1]This work is supported by the U.S. Department of Energy and the JDRD Program at the University of Tennessee.

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Date submitted: 20 Nov 2008 Electronic form version 1.4