Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First-Principles Study of Atomistically Engineered 2D-Boron Sheets KAH CHUN LAU, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI — Based on density functional theory with a planewave basis set, the stability, morphology and electronic properties of 2D boron sheets are studied. We suggest that a 2D boron sheet can be stable, and can posses metallic, half-metallic and semiconducting properties, depends on their distinct configurations. In contrast to previous studies, we predict the stability of a new novel 2D reconstructed {1221} boron sheet over the idealized {1212} triangular plane, together with their corresponding buckled configurations. Despite the high stability in cohesive energy, the unique features in geometry and electronic properties found in both configurations, suggest strong variations in electronic and mechanical properties, which might occur when the plane is rolled into different chiral structures of single-wall boron nanotubes.

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Date submitted: 11 Jan 2006 Electronic form version 1.4