Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electronic Properties of XB_6 rods: a theoretical study[1] GUANGPING LI, JING LU, R.F. SABIRIANOV, W.N. MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, C.L. CHEUNG, X.C. ZENG, Department of Chemistry, University of Nebraska - Lincoln, Lincoln, NE 68588 — Metal hexaborides have varieties of interesting properties and are utilized frequently in technological applications: LaB_6 has low work function (WF=2.6 eV), and is used as electron emitter. Experiments indicated LaB_6 nanorods generate stronger electric current than in the bulk case. We focus on the electronic structure of quasi-1D XB_6 nanorods (X = Si, Ca, Sr, Y, Ba, and most of the rare earth elements) with various widths and breadths for studying the relationship between WF and rod shape by using density functional theory with many-body and relativistic effect included included. Then the electronic structure properties such as Fermi energy and and electrostatic potential are calculated to deduce the work function. Cluster model with several cross section areas is used to investigate the size dependence of ionization potential which is found to decrease with the increasing number of unit cells: 3.3 eV for 1-cell and 2.7 eV for 6-cell cluster. The trend is in reasonable agreement with the experimental studies.

[1]This work is supported by Nebraska Research Initiative.

Guangping Li
Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182

Date submitted: 25 Nov 2007 Electronic form version 1.4