Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Electronic and transport properties of metallic hexaboride nanorods LU WANG, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, DANIEL VALENCIA, JUN-QIANG LU, Department of Physics, University of Puerto Rico at Mayagüez, PR 00681, RENAT SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588 — In this work, we performed electronic structure calculations of quasi one-dimensional metallic hexaboride XB_6 nanorods, where X are mostly rare-earth metals with $4f$ levels such as La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu, which usually regarded as good thermoelectric materials because of their low work functions and transport properties. Our purpose is to facilitate the research and manufacture of metal boride probes, thus we study extensively the size-dependence and element-specificity of the electronic properties. In these nanorods, we uncovered few general features that elucidate their excellent thermionic and field emission property. To further investigate the transport properties, we adopted the combined Landauer-Buttiker formalism and non-equilibrium Green's function technique to compute the transmission coefficients near the Fermi level and found that hexaboride nanorods can be converted from metallic to semiconducting by applying a gate voltage larger than 10 V.

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Date submitted: 06 Dec 2011 Electronic form version 1.4