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Electronic Properties and Work Functions of Metallic Hexaboride Rods and Slabs LU WANG, GUANGFU LUO, RENAT F. SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, JING LU, Mesoscopic Physics Laboratory, Department of Physics, Peking University, Beijing 100871, P. R. China, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln NE 68588-0416 — 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. In addition we included Ca, Sr, Ba, Sc, Y, and Si for comparison and then complimented those with calculations of LaB6 slabs with different boundaries and low index surfaces. 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, particularly the work functions, in nanorods and slabs composed of the rare-earth metal borides, which usually regarded as good thermoelectric materials. We uncovered few general features that elucidate their excellent thermionic and field emission property. To accomplish our calculations, we applied density functional theory together with minimization scheme based on the ensemble density functional theory to facilitate convergence when optimizing structures of these rare-earth metallic haxaboride rods, which have plenty of 4f levels at the Fermi levels.

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