

Abstract Submitted
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Electronic properties of 1D LaB₆ rods¹ G. P. LI, W. N. MEI, JING LU, R. F. SABIRIANOV, Department of Physics, University of Nebraska at Omaha, C. L. CHEUNG, X. C. ZENG, Department of Chemistry, University of Nebraska-Lincoln — Metal hexa-borides have varieties of interesting properties and were utilized frequently in technological applications: e.g. LaB₆ is known to have extremely low work function, thus is used as one of the most popular electron emitter. Our project is initiated by the experimental findings that LaB₆ nano-rods generated stronger electric current than in the bulk case. Thus we focus on the band structure calculations of quasi-1D nano-rods with various widths and breadths for the purpose of studying the relationship between work function and rod shapes. Our samples consist of up to ten unit cells, i.e. $n\mathbf{a} \times m\mathbf{b}$ (\mathbf{a} and \mathbf{b} are lattice vectors and $n \times m \leq 10$). To accomplish our calculations, we applied GGA density functional theory with all electron and relativistic effect included.

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