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Work functions and transport properties of finite metallic hexaboride nanorods LU WANG, GUANGFU LUO, RENAT F. SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, DANIEL VALENCIA, CARLOS H. SIERRA LLAVINA, JUN-QIANG LU, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, Mayaguez, PR 00680, CHIN LI CHEUNG, Department of Chemistry University of Nebraska-Lincoln, Lincoln, NE 68588 — We performed density functional theory calculations of finite metallic hexaboride LaB_6 nanorods, which are regarded as good thermoelectric materials for their low work functions. Our purpose is to facilitate the research and manufacture of metal hexaboride probes, thus we study extensively the work functions and electron transport properties of these finite nanorods. The work functions were deducted from the calculated electrostatic potential and the Fermi energy. We found that these finite LaB_6 nanorods have low work functions similar to their infinite counterpart. To further investigate the electron 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 the finite LaB_6 nanorods can be converted from metallic to semiconducting by applying a gate voltage larger than 10 V.

Wai-Ning Mei
Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182

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