Abstract Submitted
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Theoretical studies of the electronic and transportation properties of Gd disilicide nanowires on Si(001)[1] WENJIE OUYANG, YANNING ZHANG, University of California, Irvine, SHENGYONG QIN, ANPING LI, Oak Ridge National Lab, RUQIAN WU, University of California, Irvine — The scanning tunneling microscopy data demonstrate the successful growth of isolated $GdSi_2$ nanowires and wire bundles on Si (100) surface and the nano transport measurement shows the isolated nanowires exhibit a metal-insulator transition (MIT) upon cooling while the wire bundles maintain a metallic state. We investigate the structural and electronic properties of isolated $GdSi_2$ nanowires and wire bundles surface through extensive density functional calculations. A 8aSi-wide supercell was used to mimic the environment of a single nanowire, and a 5aSi-wide supercell was used for wire bundles. Interestingly, we found that the bundle structures frustrate the Perils-type structural transition that occurs easily in single nanowires. This can be regarded as the reason for the observed MIT. We also explored the effect of Si adatoms on top of wires and wire bundles. The electrical transport behaviors of $GdSi_2$ nanowires are further explained using the calculated local electronic density of states and band structures. The special magnetic ordering and its effect on other properties of nanowires will also be discussed.

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