Abstract Submitted
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Understanding the behavior of buried Bi nanostructures from first principles[1] HUNTER SIMS, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Lab, JIAMING SONG, BETHANY HUDAK, ANDREW LUPINI, PAUL SNIJDERS, Oak Ridge National Lab — Bismuth dopants in silicon provide several advantages over other n-type options such as phosphorus for usage as quantum bits (qubits). Self-assembled Bi nanolines on Si (100) surfaces may provide a means of introducing these dopants with greater control over placement and with less damage to the host system than is possible using ion implantation. However, these structures have thus far only been observed in vacuum, limiting their usefulness for application. We examine Bi nanolines overgrown with amorphous Si using density functional theory, comparing our findings with observations from scanning tunneling microscopy (STM) and atomic-resolution scanning transmission electron microscopy (STEM) in order to better understand the way in which the Si surface is influenced by both the Bi ad-dimers and the capping layer. We compare the thermodynamic stability of the generally accepted haiku defect core to the modified core that we observe and offer insight from total energy calculations into how the overgrowth process affects the nanolines.

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