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**Investigation of surface reconstructions in [110] Ge nano-wires.**[1]
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— It is anticipated that nano-structures will lead to the development of novel optical devices. It is known that quantum confinement transforms indirect band-gap crystals into direct band gap nano-structures. Although is it predicted that Ge [110] nano-wires will have a direct band gap, the optical absorption spectra has yet to be measured for free standing Ge nano-wires. Recent calculations have focused on investigating the HOMO-LUMO gap in hydrogenated Ge nano-wires. (1) This surface passivation technique neglects surface states, which are suspected to be the primary recombination mechanism in these Ge nano-structures. Here we investigate the surface reconstructions of [110] Ge nano-wires using the real-space density functional theory formalism encoded in the PARSEC software. (2) The structure and electronic states associated with wires as large as 1.2 nm diameter are investigated. Simulated annealing is used to identify the minimum energy structure out of the many possible reconstructions. (1) S. P. Beckman, Jiaxin Han, and James R. Chelikowsky. Phys. Rev. B. 74, 165314 (2006). (2) http://www.ices.utexas.edu/parsec/

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