Abstract Submitted
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In-Rich Reconstructions of the InSb(100) Surface and Chemisorption of Lithium on the c (8x2) Surface - An Ab Initio Study.* SRIDEVI L. GANAPATHY, A. K. RAY, Physics Department, The University of Texas at Arlington,76019 — The local density approximation to density functional theory (LDA-DFT) has been used to study the different possible relaxations and reconstructions of the In-rich InSb (100) surface. The surfaces are modeled by a three-layer surface with alternating In and Sb atoms and In atoms in the first layer. Hydrogen atoms are used to saturate the dangling bonds of In atoms in the bottom layer to simulate the semi-infinite effect of the surface. Periodic boundary conditions with pseudo-potentials have been used and all simulations have been carried out with the Gaussian 03 suite of programs.[1] We will report on various electronic and geometric structure properties of the possible (1x2), (2x1), (4x2) and c (8x2) reconstructed surfaces. We will also report our studies on adsorption of Li in the most symmetric sites of c (8x2) surface. Details of the chemisorption process, such as the adsorption energies, adatom separation distances, charge distributions, density of states, will be presented and compared with available results in the literature. Possible changes in the InSb surface due to Li adsorption will also be discussed in detail. *Work supported, in part, by the Welch Foundation, Houston, Texas (Grant No. Y-1525). [1] *Gaussian03*, M. J. Frisch *et al.*, Gaussian Inc., Pittsburgh, PA.

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