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A First-principles Study of GaSb(001) Surface Reconstruction SEONG-GON KIM, JEFFERY HOUZE, SUNGHO KIM, Mississippi State University, STEVEN C. ERWIN, Naval Research Laboratory — We use total-energy and electronic structure calculations based on density functional theory to study the structure of GaSb(001) growth surfaces. We consider different reconstruction models proposed in the literature on the basis of experimental observations under typical GaSb growth conditions and present the T=0 surface stability diagram. We found that all  $(n \times 5)$ -like reconstructions proposed in various literature have too high surface formation energies to adequately model the structures observed experimentally under typical Sb-rich growth conditions. We found several new reconstruction models for GaSb(001) surface with correct symmetries that have lower surface formation energies than existing models and produce correct STM images.

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