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The atomistic mechanism for Sb segregation and As displacement of Sb in InSb(001) surfaces

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Highlights

- Atomistic mechanisms for observations of As-for-Sb exchange and Sb segregation
- *ab initio* calculations of pure and As-exposed InSb(001) surface reconstructions
- A predicted phase diagram for pure InSb is in better agreement with experiments
- Experiments and calculations show the A-(1x3) consists of multiple reconstructions

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