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Theoretical Phase Stability of Silicon Nanomembranes Under Pressure JOEL AMBRIZ PONCE, WILLIAM PARKER, University of Wisconsin - Parkside — The wide range of applications of semiconducting silicon surround us in electronic, optical, and mechanical devices.Flat, tens-of-nanomemter-thick membranes of pure silicon can now be synthesized and thickness-dependence changes in membrane properties have been reported.To understand and predict the evolution of these properties, we model atomistic silicon slabs at the electronic level using density functional theory at varying levels of exchange-correlation functional. In particular, we investigate the pressure-based transition from the ambient-condition diamond phase to the higher-pressure beta-tin phase under compression both uniaxially out-of-plane uniaxial and biaxially in the plane of the membrane. We calculate the transition pressure and volume as well as the elastic properties of each phase at varying slab thicknesses.

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