

Abstract Submitted
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Where is the Simple Hexagonal Structure in Tin?¹ MICHAEL MEHL, DANIEL FINKENSTADT², Naval Research Laboratory — The heavier elements of periodic table column IV exhibit number of structural phase transitions under pressure. Si and Ge transform from the ground-state diamond structure to, successively, the β -Sn structure, a body-centered orthorhombic structure, the simple hexagonal structure, etc., ending at a close-packed phase (fcc or hcp) near 200 GPa. Tin also transforms from diamond to β -Sn, but then to a body-centered tetragonal phase, ending with the body-centered cubic phase. The simple hexagonal phase is not seen, despite the fact that numerous tin-rich alloys exhibit a simple hexagonal structure. To understand this we performed DFT calculations on tin in various crystal structures, using both full-potential LAPW and VASP with a PAW potential. Surprisingly, we find that the simple hexagonal phase is degenerate with β -Sn over pressures at which the β -Sn phase is seen experimentally. This holds both for LAPW and VASP calculations, in both the LDA and the GGA. We explore reasons for the lack of a tin simple hexagonal phase, including zero point and spin-orbit effects.

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