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Growth conditions of oxypnictide compounds LaFePnO Pn={P,As,Sb} JASON VIELMA, SEAN MUIR, M.A. SUBRAMANIAN, A.W. SLEIGHT, GUENTER SCHNEIDER, Oregon State University — The discovery of superconductivity in layered ferro-oxynictides LaFePO ($T_c \sim 4\ K$) and $LaFeAsO_{1-x}F_x$ ($T_c \sim 26\ K$) lead to an intense search for other iron based superconducting materials. For the hypothetical compound LaFeSbO, ab initio density functional theory (DFT) calculations predict an enhanced density of states at the Fermi level together with increased nesting between the electron and hole sheets in the tetragonal structure (isostructural to LaFeAsO) and an enhanced spin-density wave ground state in a closely related orthorhombic structure; indicating the potential for superconductivity with a higher transition temperature [1]. We report ab initio DFT calculations of the phase stability of the oxypnictides LaFePnO Pn={P,As,Sb} and find growth conditions where LaFePO and LaFeAsO are thermodynamically stable, but LaFeSbO is unstable with respect to the formation of La_2SbO_2. Indeed, our attempt to synthesize LaFeSbO led to the synthesis and characterization of La_2SbO_2. The phonon spectrum of hypothetical LaFeSbO shows no soft modes, indicating that LaFeSbO is potentially metastable and leaving open the possibilty of a nonequilibrium synthesis route.

[1] C-Y. Moon, S. Y. Park, and H. J. Choi, Phys. Rev. B, **78**, 212507 (2008)

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