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Prediction of novel thermodynamically stable lithium-tin binary compounds at ambient and high pressure. RAJA SEN, PRIYA JOHARI, Department of Physics, School of Natural Sciences, Shiv Nadar University, India. — Volume expansion and elastic softening of Sn anode on lithiation result in mechanical degradation and pulverization of Sn, affecting the overall performance of Li-Sn batteries. It can however be overcome by using exotic high pressure quenched phases as prelithiated reagent. Under pressure many unusual stoichiometry which are basically impossible at ambient pressure, can be synthesized, which may even survive the decompression from high to ambient pressure. We therefore have performed first-principles evolutionary algorithm based simulations to explore the phase diagram of Li-Sn compounds in the pressure range of 1 atm-20 GPa. Besides the well-known existing Li-Sn compounds, our studies reveal the existence of five unreported stoichiometry (Li_8Sn_3, Li_3Sn_1, Li_4Sn_1, Li_5Sn_1, and Li_7Sn_1) at ambient and high pressure. While Li_8Sn_3 has been identified as one of the most stable Li-Sn compound in the entire pressure range, the pressure induced Li-rich compounds like Li_5Sn_1 and Li_7Sn_1 have been classified as providing higher theoretical gravimetric capacity of 1129 and 1580 $mAhg^{-1}$, respectively.

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