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Ab-initio structure prediction and electronic properties of $[Si_xSn_{1-x}]_3N_4$ ternary nitrides

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Abstract: Group IV-Nitrides with spinel structures i.e. γ-M_3N_4 (M= Si,Ge,Sn) exhibit electronic bandgaps which span the visible spectrum making them suitable for optoelectronic devices. $[Si_xSn_{1-x}]_3N_4$ is the most challenging ternary compound, with a bandgap tunable over a broad area. The USPEX evolutionary structure prediction code interfaced with the VASP code is used in order to predict the structure of Sn_3N_4. The energetically preferable is found to be the spinel structure, while the second best is the hexagonal β-Si_3N_4-like structure. Following these results, an in depth analysis of the $[Si_xSn_{1-x}]_3N_4$ ternary alloy is performed, resulting in the preferable atom configurations for both cubic and hexagonal $[Si_xSn_{1-x}]_3N_4$ for the full range of x. The cubic structure is found to be preferable for small Si content, but before x=0.33 a switch to the hexagonal structure occurs. Finally, hybrid functional calculations are employed to accurately construct the bandstructures of all the examined configurations and the corresponding bandgaps are calculated. A quadratic fit is applied and the bowing parameters of the bandgaps for both structures are extracted.