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Structural and thermochemical Aspects of (III-V)IV_3 Material Assembly from First Principles[1] ANDREW CHIZMESHYA, JOHN KOUVETAKIS, Arizona State Univ — Alloys with (III-V)-(IV) compositions, including $Si_3(AlP)$, $Si_{5-2y}(AlP)_y$, $Si_3Al(As_{1-x}N_x)$, $Si_{5-2y}Al(P_{1-x}N_x)_y$ and $Ge_{5-2y}(InP)_y$ and have recently been synthesized as mono-crystalline films on Si substrates, using a synthesis route specifically designed to avoid phase separation between the III-V and IV constituents. Molecular "building blocks" containing group-V-centered III-V-IV_3 cores, formed via interactions of group-III atoms and reactive silyly/germyl hydride precursors of desired composition (e.g, $P(SiH_3)_3$, $P(GeH_3)_3$, etc), assemble to form stable, covalent, diamond-like materials with the inherent tetrahedral symmetry and composition of the III-V-IV_3 units. The resulting systems may provide access to a broad range of new semiconductor systems with extended optoelectronic properties, provided that the required molecular sources are available, the thermodynamic processes are viable, and the resulting alloy composition can be tuned to lattice-match the growth substrate. Molecular/solid-state simulations are used to identify promising synthetic pathways and guide the epitaxial creation of new (III-V)-(IV) materials. The thermodynamics of gas phase synthesis reactions, energetic stability of the alloys, and their epitaxial/chemical compatibility with the substrate are combined to form a global figure of merit. The latter corroborates the synthesis of known systems and predicts that formation of $GaPSi_3$/Si(100), $GaAsSi_3$/SiGe(100), $AlPGe_3$/Ge(100) and $InAsSi_3$/Ge(100) may also be favorable.

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