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First-principles study of non-isovalent Si-III-V and Si-II-VI alloys: Covalent, ionic and their mixed phases

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Obtaining optically active Si-based materials is a considerable challenge that holds great potential for optoelectronics and solar energy conversion with silicon. Of the progress that has been made in recent years, one of the promising methods is to make use of molecular precursors for the non-equilibrium growth of non-isovalent Si-III-V alloys such as Si_3AlP. In this paper, we propose a new class of non-isovalent Si_2AlP (or Si_2ZnS) alloys as a unique material system with tunable local chemical orders around Si atoms within the same composition and structural motif. The proposed alloys can thus be used for systematically studying different prototypes of non-isovalent alloys with "covalent", "ionic", and "mixed" local environments. Using first-principles hybrid functional calculations, we discuss how the local chemical orders affect the electronic and optical properties of the non-isovalent alloys. We also identify a direct-bandgap Si_2ZnS phase with strong absorption in the visible range.