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A first-principles study on second-order ferroelectric phase transition in two-dimensional puckered group V materials. SANG-HOON LEE, SEUNG-HOON JHI, POSTECH — We study two-dimensional group V materials (P, As, Sb, and Bi) in puckered honeycomb structure using first-principles calculations. Two factors, the degree of puckering and buckling characterize not only the atomic structure but also the electronic structure and its topological phase. By analyzing the lone-pair character of constituent elements and the softening of the phonon mode, we clarify the origin of the buckling. We show that the phonon softening leads the second-order type structural phase transition from a flat to a buckled configuration. The inversion symmetry breaking associated with the structural transition induces the spontaneous polarization in these homogenous materials. Our calculations suggest that external strains or n-type doping are effective methods to control the degree of buckling. We find that the ferroelectric and non-trivial topological phase can coexist in puckered Bi when tensile strains are applied.

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