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Half-layer-by-half-layer growth of a blue phosphorene monolayer on the GaN(001) substrate[1] JIANG ZENG[2], PING CUI, ZHENYU ZHANG, Univ of Sci Tech of China — Black phosphorene (BlackP), consisting of a vertically corrugated yet single layer of phosphorus atoms, is a latest member of the expanding two-dimensional (2D) materials family with high carrier mobility and immense application potentials. Blue phosphorene (BlueP), an allotrope of BlackP with appealing properties of its own, consists of a more flatly arranged layer of phosphorus atoms. To date, direct growth of either BlackP or BlueP remains a daunting challenge. Using first-principles approaches, here we establish a novel kinetic pathway for fabricating BlueP via epitaxial growth. Our systematic energetic studies reveal that both BlackP and BlueP monolayers can be readily stabilized on Cu(111), Au(111), and GaN(001) substrates, but with contrasting thermodynamic stabilities. The semiconducting GaN(001) is further shown to be superior for fabricating BlueP, through an intriguing half-layer-by-half-layer (HLBHL) growth mechanism. Within this scheme, the GaN(001) surface is first preferentially covered by a half layer of phosphorus adatoms, followed by the addition of the other half. Once formed, such a BlueP monolayer is thermodynamically stable, as tested using *ab initio* molecular dynamics simulations.

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