A novel two-dimensional beryllium diphosphide (BeP_2) with superconductivity: the first-principles exploration

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S1. The optimized structure parameters, the relative energy in four BeP_2 structures.

Table S1. The optimized structure parameters a, b (Å), <**a**,**b**> vector angle (X°), and relative energy (eV per atom), the energy reference point is set as BeP_2-1 with the lowest energy.

	a	b	<a, b>	Energy (eV per atom)
BeP_2-1	**3.76**	**5.22**	**111**	**0.0**
BeP_2-2	**6.07**	**3.6**	**90**	**0.009**
BeP_2-3	**3.61**	**5.8**	**90**	**0.017**
BeP_2-4	**6.59**	**8.68**	**67.68**	**0.088**

S2. Geometric atomic configurations for four BeP_2 configures with small virtual frequency at gamma point.

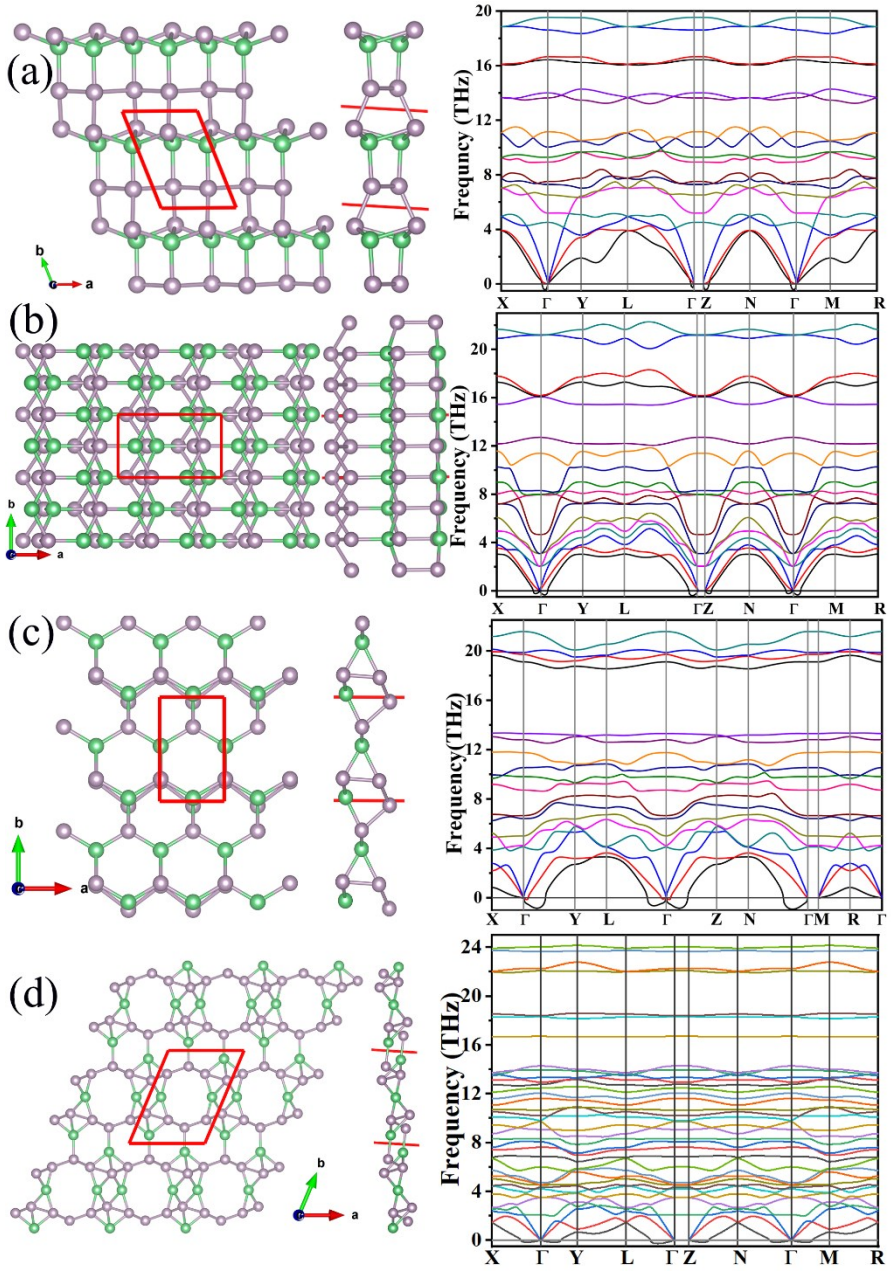

Fig. S2. Geometric atomic configurations of the predicted layer (left panel), side views (middle panel), phonon spectra (right panel) of 2D (a) BeP_2-1, (b) BeP_2-2, (c) BeP_2-3, (d) BeP_2-4.

S3. The band structure of 2D 1H-BeP_2 with vdw/SOC/HSE06

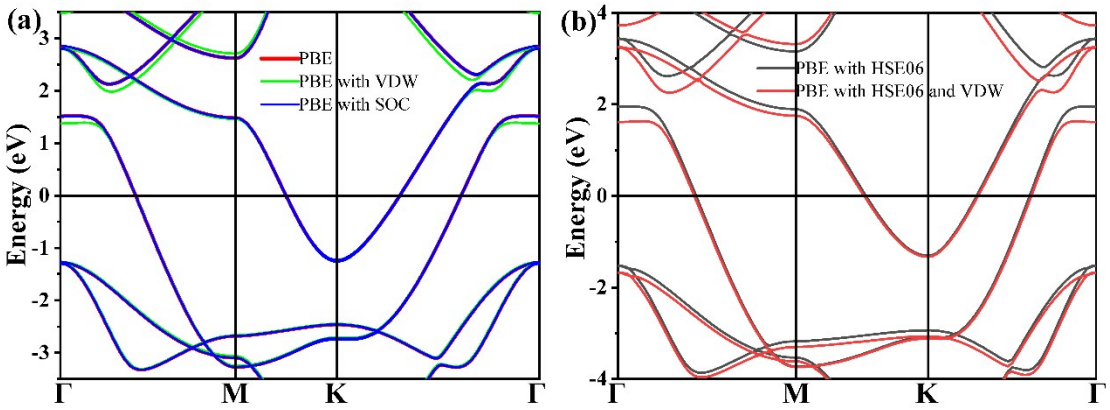

Fig. S3. The band structures of 1H-BeP_2 by (a) PBE without and with VDW or SOC. (b) PBE with HSE06 or HSE06 and VDW.