

Supplementary Information for

Epitaxial growth of a buckled BiP monolayer on Bi(111)

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Supplementary Table 1 –2.

We performed additional calculations using GGA, DFT-D2, vdW-DF, vdW-DF2, and optB88-vdW. All six configurations in Fig. 5 were fully relaxed with each functional. The calculated total energies are summarized in Table S1, and the corresponding relative energies are shown in Table S2.

Table S1. Total energies (in eV/unit cell) of the six adsorption configurations shown in Fig. 5, calculated with GGA and five different vdW-inclusive functionals.

Config.	GGA	DFT-D2	DFT-D3	vdw-DF	vdw-DF2	optB88-vdW
1	-32.42312	-33.89073	-30.60514	-18.07545	-4.04376	-4.14387
2	-32.51655	-33.88839	-30.70673	-20.32543	-4.10329	-4.3142
3	-32.26287	-33.64602	-30.45567	-13.38278	-4.05406	-4.22021
4	-32.48778	-33.94519	-30.64656	-20.86983	-4.16809	-4.2457
5	-32.53641	-33.94659	-30.71641	-21.14078	-4.16753	-4.45218
6	-32.32789	-33.82234	-30.51778	-20.05681	-4.10377	-4.33261

Table S2. Relative energies (in eV/unit cell) of the six adsorption configurations, referenced to Config 5 for each functional. Values are derived from the total energies in Table S1.

Config	GGA	DFT-D2	DFT-D3	vdw-DF	vdw-DF2	optB88-vdW
1	0.11329	0.05586	0.11127	3.06533	0.12377	0.30831
2	0.01986	0.05820	0.00968	0.81535	0.06424	0.13798
3	0.27354	0.30057	0.26074	7.75800	0.11347	0.23197
4	0.04863	0.00140	0.06985	0.27095	-0.00056	0.20648
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.20852	0.12425	0.19863	1.08397	0.06376	0.11957