Supporting Information for

Tunable band gap of graphyne-based homo- and hetero-structures by stacking sequences, strain and electric field

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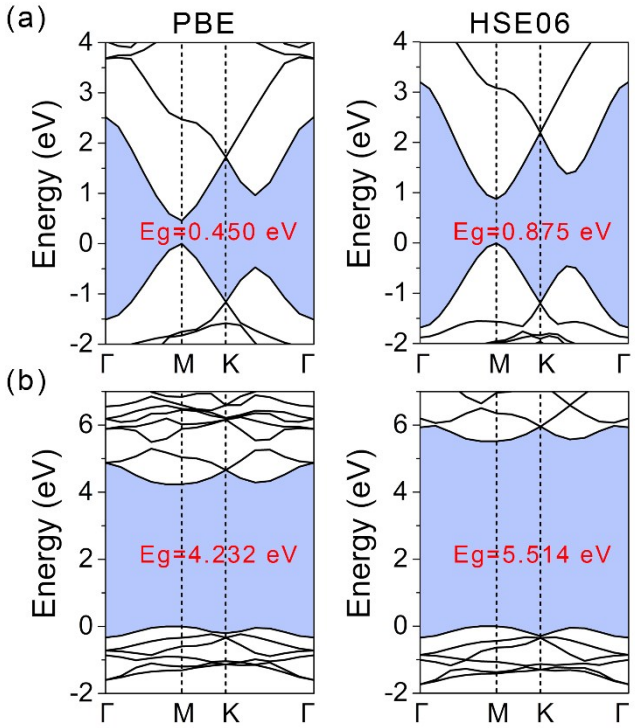

Fig. S1 Calculated BS of (a) Gyne and (b) BNyne monolayer based on PBE and HSE06 functionals, respectively.

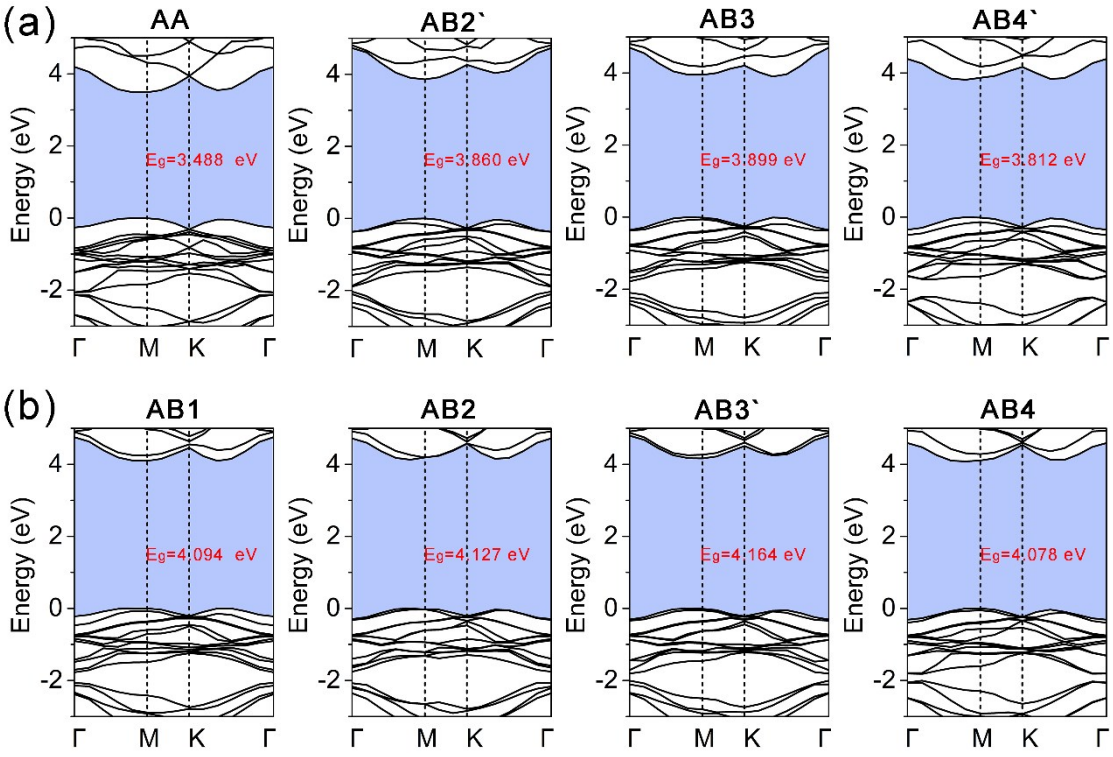

Fig. S2 Calculated BS of (a) group I and (b) Group II BNyne/BNyne bilayers

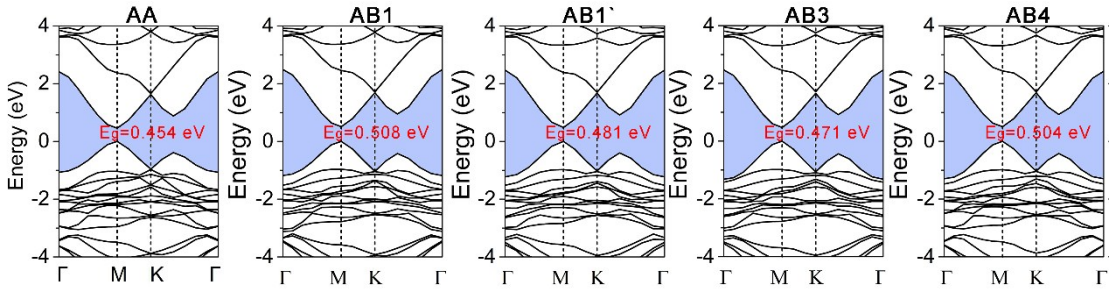

Fig. S3 Calculated BS of Gyne/BNyne bilayers

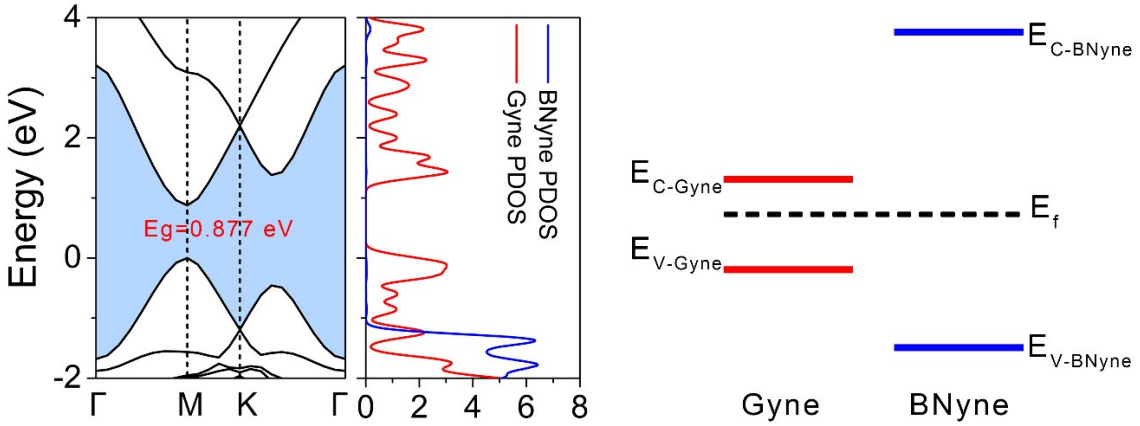

Fig. S4 Calculated BS, PDOS and corresponding band offset diagrams of AB2-Gyne/BNyne based on HSE06 hybrid functional.

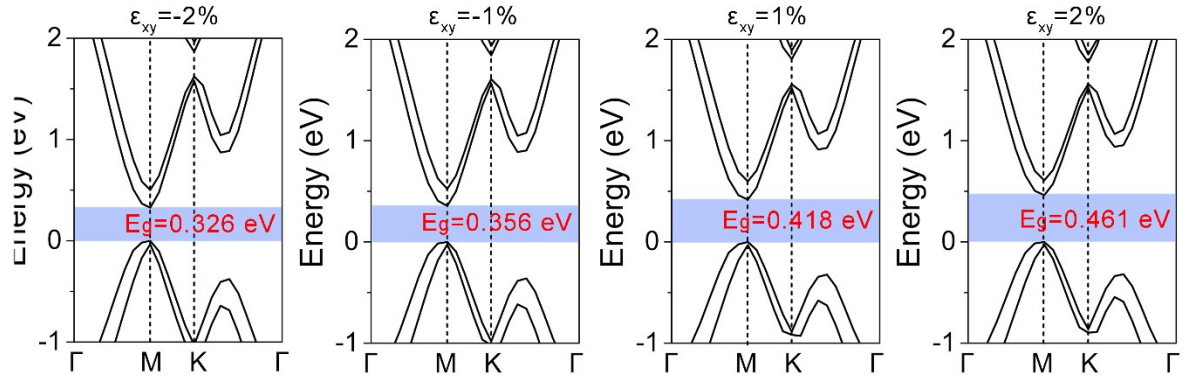

Fig. S5 Calculated BS of the AB1-Gyne/Gyne bilayer under biaxial strain of ε_{xy}=-2%, -1%, 1% and 2%, respectively.

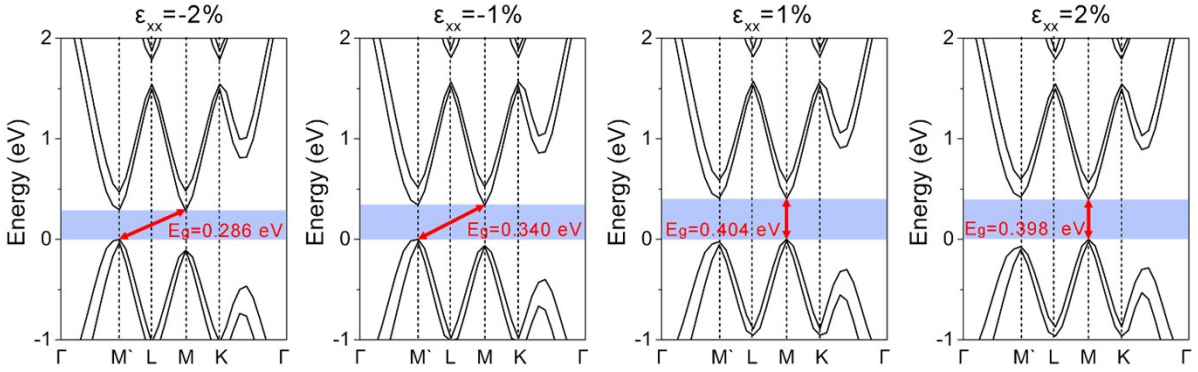

Fig. S6 Calculated BS of the AB1-Gyne/Gyne bilayer under uniaxial strain of ε_{xx}=-2%, -1%, 1% and 2%, respectively.

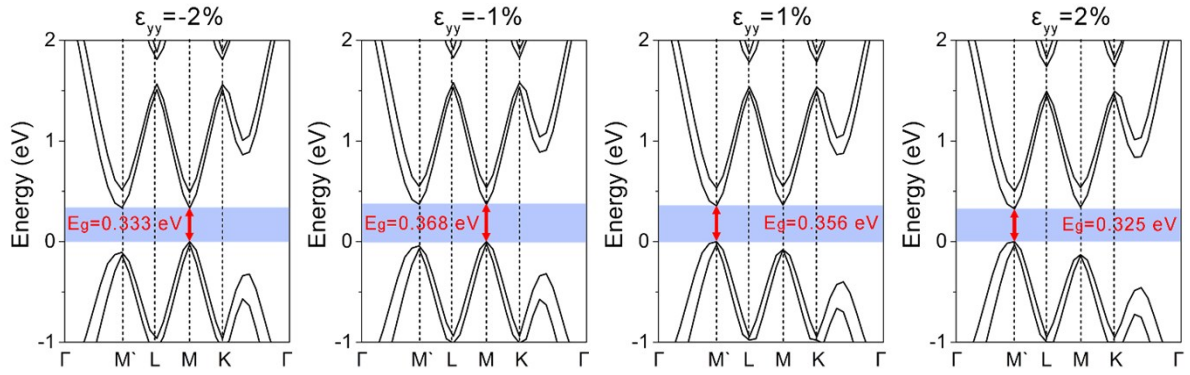

Fig. S7 Calculated BS of the AB1-Gyne/Gyne bilayer under uniaxial strain of ε_{yy}=-2%, -1%, 1% and 2%, respectively.

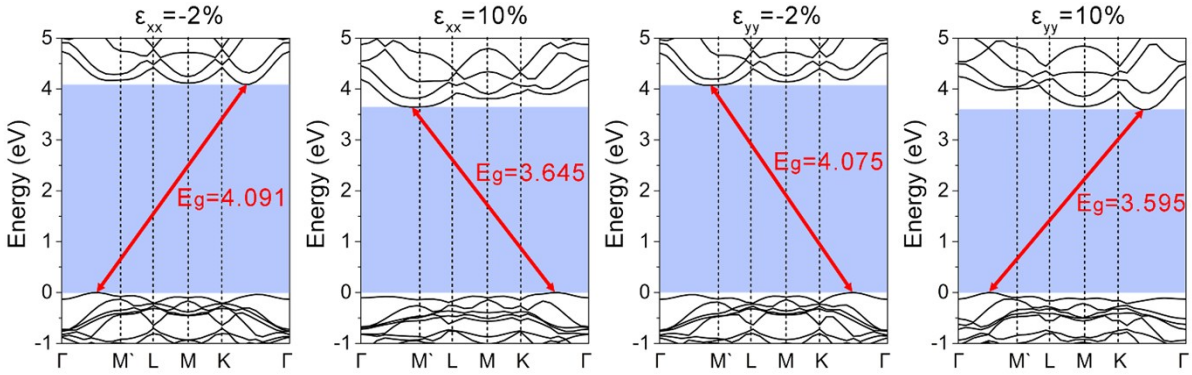

Fig. S8 Calculated BS of AA`-BNyne/BNyne under ε_{xx}=-2%, 10% and ε_{yy}=-2%, 10%, respectively.

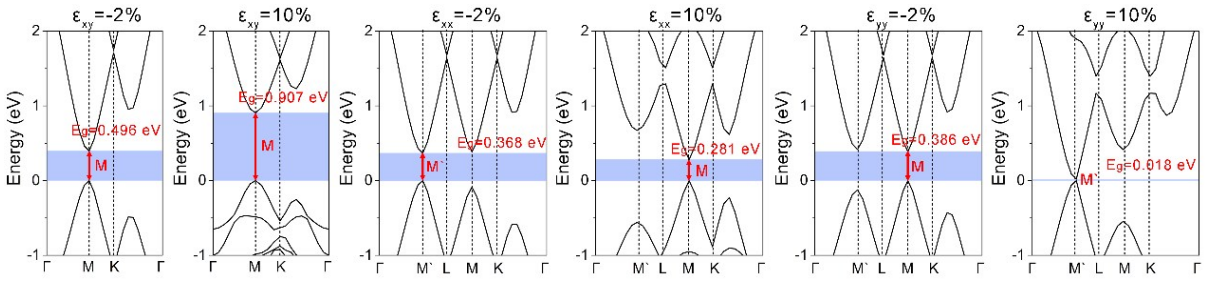

Fig. S9 Calculated BS of Gyne/BNyne bilayers under strain

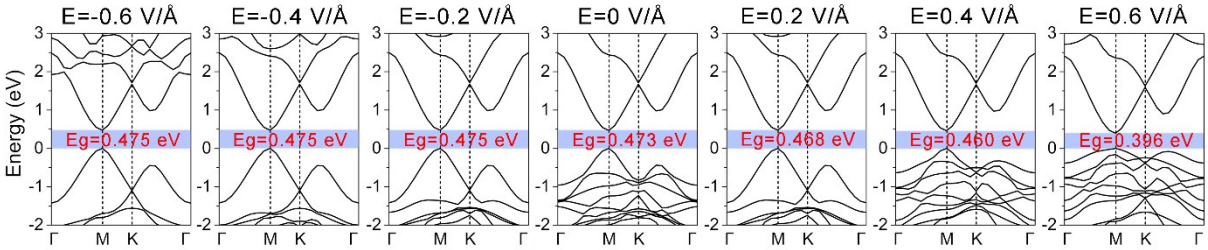

Fig. S10 Calculated BS of Gyne/BNyne bilayers under external electric field

Table S1 Calculated positions of conduction band minimum (CBM) and valence band maximum (VBM) and band gap values Eg (unit: eV) of AB1-Gyne/Gyne with ε_{xy}, ε_{xx} and ε_{yy}.

Strain	-2%	-1%	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
ε_{xy}												
Eg	0.326	0.356	0.418	0.461	0.494	0.531	0.568	0.612	0.653	0.700	0.750	0.801
CBM	M	M	M	M	M	M	M	M	M	M	M	M
VBM	M	M	M	M	M	M	M	M	M	M	M	M
ε_{xx}												
Eg	0.286	0.340	0.404	0.398	0.390	0.376	0.360	0.339	0.315	0.286	0.256	0.228
CBM	M	M	M	M	M	M	M	M	M	M	M	M
VBM	M`	M`	M	M	M	M	M	M	M	M	M	M
ε_{yy}												
Eg	0.333	0.368	0.356	0.325	0.292	0.259	0.221	0.186	0.156	0.124	0.112	0.079
CBM	M	M	M`	M`	M`	M`	M`	M`	M`	M`	M`	M`
VBM	M	M	M`	M`	M`	M`	M`	M`	M`	M`	M`	M`

Table S2 Calculated positions of CBM and VBM and band gap values Eg (unit: eV) of AA`-BNyne/BNyne with ε_{xy}, ε_{xx} and ε_{yy}.

Strain	-2%	-1%	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
ε_{xy}												
Eg	4.211	4.152	4.038	3.978	3.918	3.860	3.804	3.748	3.693	3.639	3.584	3.525
CBM	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M
VBM	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M	Γ-M
ε_{xx}												
Eg	4.091	4.098	4.042	3.990	3.939	3.890	3.849	3.804	3.762	3.722	3.682	3.645
CBM	Γ-K	Γ-K	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`
VBM	Γ-M`	Γ-M`	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K
ε_{yy}												
Eg	4.075	4.085	4.039	3.981	3.924	3.873	3.820	3.770	3.722	3.677	3.635	3.595
CBM	Γ-M`	Γ-M`	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K	Γ-K
VBM	Γ-K	Γ-K	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`	Γ-M`

Table S3 Calculated positions of CBM and VBM and band gap values Eg (unit: eV) of AB2-Gyne/BNyne with ε_{xy}, ε_{xx} and ε_{yy}.

Strain	-2%	-1%	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
ε_{xy}												
Eg	0.496	0.436	0.508	0.545	0.583	0.623	0.665	0.708	0.752	0.801	0.853	0.907
CBM	M	M	M	M	M	M	M	M	M	M	M	M
VBM	M	M	M	M	M	M	M	M	M	M	M	M
ε_{xx}												
Eg	0.368	0.418	0.466	0.460	0.451	0.437	0.422	0.402	0.378	0.350	0.318	0.281
CBM	M`	M`	M	M	M	M	M	M	M	M	M	M
VBM	M`	M`	M	M	M	M	M	M	M	M	M	M
ε_{yy}												
Eg	0.386	0.428	0.437	0.398	0.353	0.310	0.265	0.215	0.164	0.113	0.061	0.018
CBM	M	M	M`	M`	M`	M`	M`	M`	M`	M`	M`	M`
VBM	M	M	M`	M`	M`	M`	M`	M`	M`	M`	M`	M`