Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Theoretical study of electronic and tribological properties of *h*-BNC_2/graphene, *h*-BNC_2/*h*-BN and *h*-BNC_2/*h*-BNC_2 bilayers

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Table S1: Cartesian coordinates of the optimized strained unit-cell of *h*-BNC_2/graphene (*I*), *h*-BNC_2/*h*-BN (*II*) and *h*-BNC_2/ *h*-BNC_2 (*III)* model systems with a fixed interlayer distance of 3.15 Å

I				*II*				*III*			
B	1.781494	1.858918	3.150000	B	1.781427	1.858917	3.150000	B	1.436828	1.858921	3.150000
N	1.045989	0.619637	3.150000	N	1.046323	0.619636	3.150000	N	0.702381	0.619639	3.150000
C	3.293453	1.858933	3.150000	C	3.292796	1.858931	3.150000	C	2.949602	1.858934	3.150000
N	7.483754	1.858924	3.150000	N	7.484263	1.858925	3.150000	N	7.140140	1.858926	3.150000
C	3.985193	0.619650	3.150000	C	3.984770	0.619648	3.150000	C	3.643546	0.619650	3.150000
C	6.104598	1.858911	3.150000	C	6.105032	1.858911	3.150000	C	5.763813	1.858912	3.150000
C	5.416613	0.619632	3.150000	C	5.416515	0.619631	3.150000	C	5.074352	0.619632	3.150000
B	8.216185	0.619645	3.150000	B	8.216344	0.619646	3.150000	B	7.871840	0.619646	3.150000
C	1.804543	1.858925	0.000000	B	1.805675	1.858920	0.000000	B	1.436828	1.858921	0.000000
C	1.088667	0.619640	0.000000	N	1.088256	0.619638	0.000000	N	0.702381	0.619639	0.000000
C	3.234111	1.858925	0.000000	N	3.234017	1.858929	0.000000	C	2.949602	1.858934	0.000000
C	7.526833	1.858927	0.000000	N	7.527582	1.858929	0.000000	N	7.140140	1.858926	0.000000
C	3.949662	0.619640	0.000000	B	3.947966	0.619648	0.000000	C	3.643546	0.619650	0.000000
C	6.095989	1.858926	0.000000	B	6.094234	1.858921	0.000000	C	5.763813	1.858912	0.000000
C	5.379310	0.619641	0.000000	N	5.380289	0.619639	0.000000	C	5.074352	0.619632	0.000000
C	8.244108	0.619642	0.000000	B	8.245012	0.619647	0.000000	B	7.871840	0.619646	0.000000
Tv	8.586000	0.000000	0.000000	Tv	8.586000	0.000000	0.000000	Tv	8.586000	0.000000	0.000000
Tv	0.000000	2.478565	0.000000	Tv	0.000000	2.478565	0.000000	Tv	0.000000	2.478565	0.000000
Tv	0.000000	0.000000	20.000000	Tv	0.000000	0.000000	20.000000	Tv	0.000000	0.000000	20.000000

Table S2: Cartesian coordinates of the optimized unstrained unit-cell of graphene, *h*-BN and *h*-BNC_2 mono-layers

Graphene				*h*-BN				*h*-BNC_2			
C	3.552500	1.845933	0.000000	B	3.564583	1.883605	0.000000	C	3.660991	1.864170	0.000000
C	2.842000	0.615311	0.000000	N	2.839583	0.627868	0.000000	C	2.958527	0.621384	0.000000
C	1.421000	0.615311	0.000000	B	1.389583	0.627868	0.000000	B	1.428584	0.621400	0.000000
C	0.710500	1.845933	0.000000	N	0.664583	1.883605	0.000000	N	0.678730	1.864183	0.000000
C	7.815500	1.845933	0.000000	B	7.914583	1.883605	0.000000	B	7.944661	1.864169	0.000000
C	7.105000	0.615311	0.000000	N	7.189583	0.627868	0.000000	N	7.199643	0.621387	0.000000
C	5.684000	0.615311	0.000000	B	5.739583	0.627868	0.000000	C	5.806178	0.621405	0.000000
C	4.973500	1.845933	0.000000	N	5.014583	1.883605	0.000000	C	5.108176	1.864190	0.000000
Tv	8.526000	0.000000	0.000000	Tv	8.700000	0.000000	0.000000	Tv	8.696222	0.000000	0.000000
Tv	0.000000	2.461244	0.000000	Tv	0.000000	2.511474	0.000000	Tv	0.000000	2.485571	0.000000
Tv	0.000000	0.000000	20.000000	Tv	0.000000	0.000000	20.000000	Tv	0.000000	0.000000	20.000000

Figure S1.- RI landscape for interlayer sliding in bilayer a) graphene (top and side view) and b) *h*-BN.

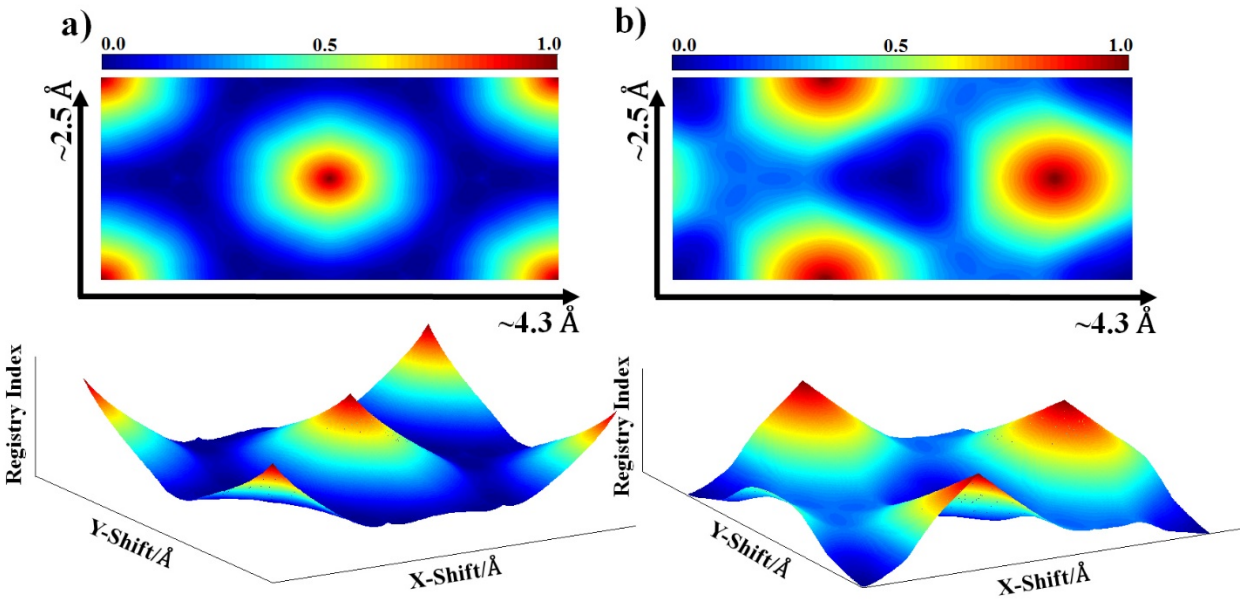

Figure S2.- (a) A finite square *h*-BNC_2 flake, (b) the center of mass of the flake corresponds to the origin of the coordinate system and (c) center of mass of the monolayer is exactly below the center of mass of the corresponding flake.