Designing of Nanoscale Capacitor Based on Twin-graphene

Jyotirmoy Deb, Harkishan Dua, Utpal Sarkar *

Department of Physics, Assam University, Silchar-788011, India

* Email: utpalchemiitkgp@yahoo.com

Supporting Information

Table S1. Calculated band gap and nature of the band gap at different electric fields of AB stacked 'twin-graphene' and single layer, double layer, triple layer 'twin-graphene like BN sheet' sandwiched between the pristine 'twin-graphene' layers.

System	Electric field (V/Å)	Band gap (eV)	Nature
AB stacked 'twin-graphene'	-1.5	0.475	Indirect band gap Semiconductor
	-1.0	0.444	Indirect band gap Semiconductor
	-0.5	0.376	Direct band gap semiconductor
	0.0	0.553	Direct band gap Semiconductor
	0.5	0.375	Direct band gap Semiconductor
	1.0	0.403	Indirect band gap Semiconductor
	1.5	0.430	Indirect band gap Semiconductor
Single layer 'twin-graphene like BN sheet sandwiched between the pristine 'twin-graphene' sheets	-1.5	-	Metallic
	-1.0	-	Metallic
	-0.5	-	Metallic
	0.0	0.694	Direct band gap Semiconductor
	0.5	-	Metallic
	1.0	-	Metallic
	1.5	-	Metallic
Double layer 'twin-graphene like BN sheet' sandwiched between the pristine 'twin-graphene' sheets	-1.5	-	Metallic
	-1.0	-	Metallic
	-0.5	-	Metallic
	0.0	0.670	Direct band gap Semiconductor
	0.5	-	Metallic

	1.0	-	Metallic
	1.5	-	Metallic
Triple layer 'twin-graphene like BN sheet' sandwiched between the pristine 'twin-graphene' sheets	-1.5	-	Metallic
	-1.0	-	Metallic
	-0.5	-	Metallic
	0.0	0.744	Direct band gap Semiconductor
	0.5	-	Metallic
	1.0	-	Metallic
	1.5	-	Metallic

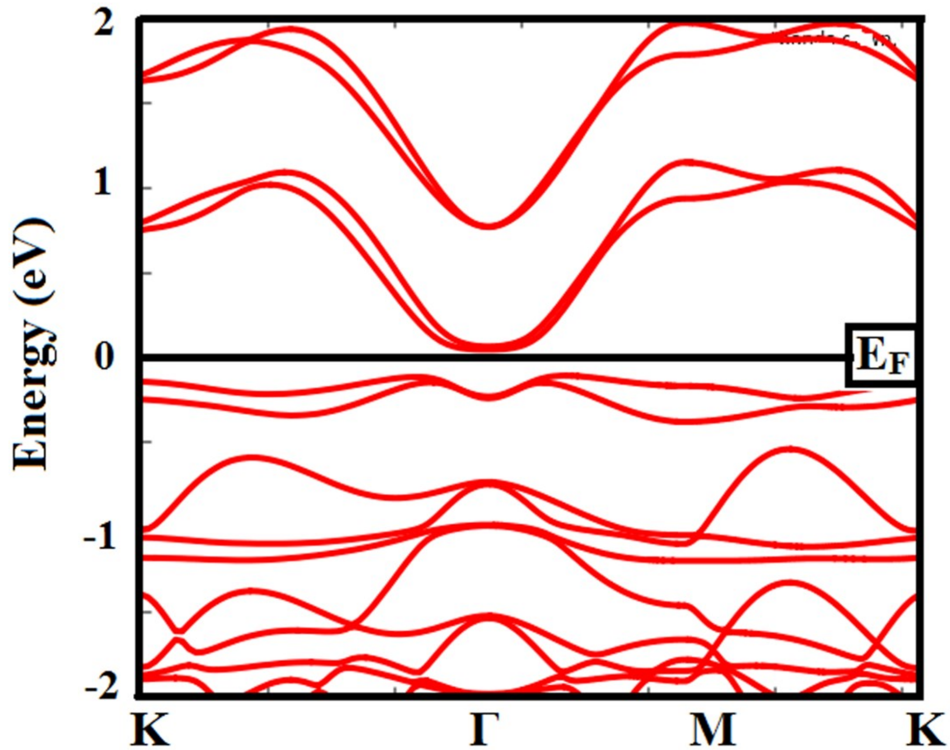

Fig. S1. Band structure of AB stacked 'twin-graphene' at electric field 1.5 V/Å.

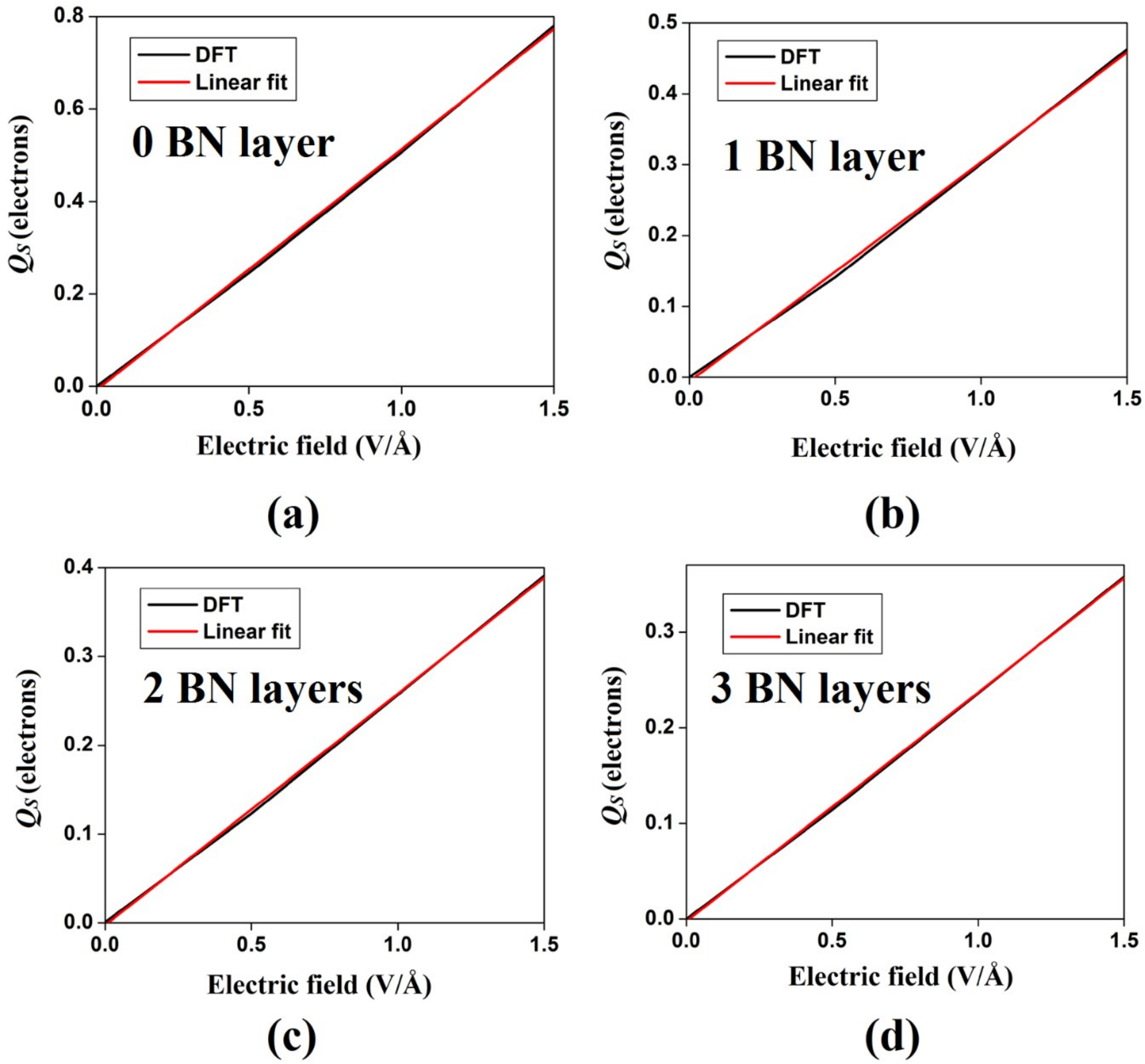

Fig. S2. Variation of the charge stored of NC and NDC models as a function of external electric field ($\vec{E}_f$) for different number of 'twin-graphene like BN sheet' sandwiched between the pristine 'twin-graphene' layers.

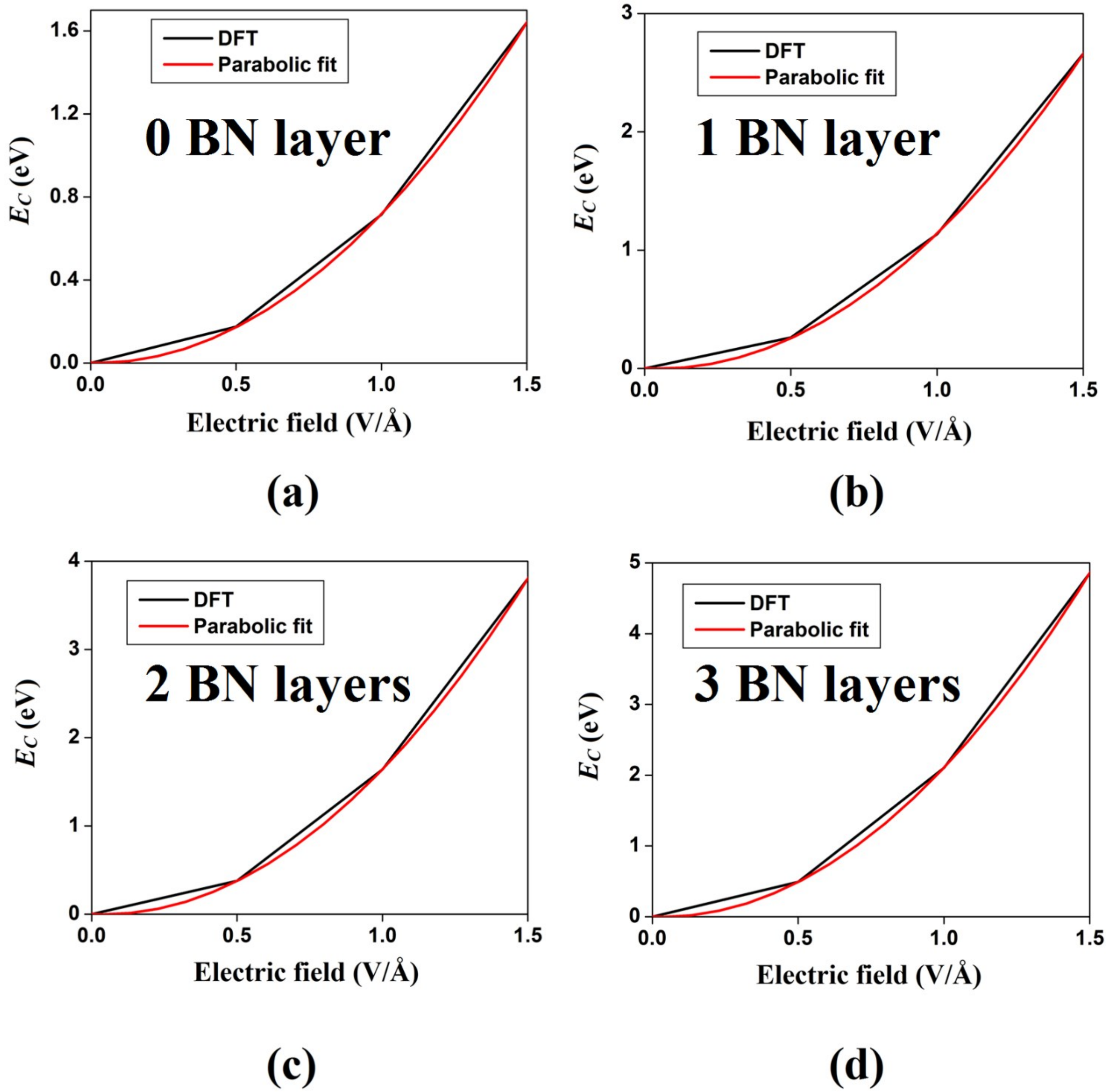

Fig. S3. Variation of the energy stored of NC and NDC models as a function of external electric field ($\vec{E}_f$) for different number of 'twin-graphene like BN sheet' sandwiched between the pristine 'twin-graphene' layers.

Table S2. Calculated interlayer distance (d), primitive unit cell mass (m), electric field ($\vec{E}_f$), dipole moment (P), charged stored (Q_s), energy stored (E_C), plane average electrostatic potential difference (ΔV_Z) and gravimetric capacitance (C_1 and C_2) of NC and NDC model for $\vec{E}_f = -1.5$ *to* 1.0 V/Å.

No. of 'twin-graphene like BN sheet' (n)	Interlayer distance (d) (Å)	Mass (m) (g) $\times 10^{-}$	Electric field ($\vec{E}_f$) (V/Å)	Dipole moment (P) (Debye)	Charged stored (Q_s) (elementary charge)	Energy stored (E_C) (eV)	Potential difference (ΔV_Z) (V)	C1 (F/g)	C2 (F/g)
0	2.887	0.718	-1.5	10.823	0.780	1.641	0.74	41.39	235.85
			-1.0	7.031	0.507	0.715	0.65	40.08	174.17
			-0.5	3.401	0.245	0.175	0.43	38.27	128.32
			0.0	0.000	0.000	0.000	0.001	0.00	1.09
			0.5	3.401	0.245	0.175	0.43	38.27	127.79
			1.0	7.031	0.507	0.715	0.65	40.08	173.77
1	8.005	1.089	-1.5	17.793	0.463	2.660	0.85	5.92	80.00
			-1.0	11.575	0.301	1.135	0.85	5.86	52.20
			-0.5	5.419	0.141	0.261	0.80	5.61	26.06
			0.0	0.004	0.000	0.000	0.01	0.00	1.39
			0.5	5.420	0.141	0.261	0.81	5.61	25.49
			1.0	11.576	0.301	1.135	0.87	5.87	51.18
2	13.368	1.460	-1.5	25.057	0.390	3.786	0.91	2.21	46.97
			-1.0	16.416	0.256	1.630	0.91	2.20	30.91
			-0.5	7.814	0.122	0.378	0.88	2.15	15.24
			0.0	0.081	0.001	0.000	0.02	0.00	7.06
			0.5	7.883	0.123	0.379	0.77	2.19	17.49
			1.0	16.483	0.257	1.639	0.80	2.20	35.21
3	18.545	1.831	-1.5	31.924	0.358	4.791	0.87	1.17	35.91
			-1.0	21.010	0.236	2.104	0.86	1.16	23.93
			-0.5	10.124	0.114	0.493	0.84	1.15	11.86

0.0	0.005	0.000	0.000	0.002	0.00	2.15
0.5	10.125	0.114	0.493	0.83	1.15	12.00
1.0	21.018	0.236	2.104	0.85	1.16	24.20