Supplementary information – Revealing the formation and electrochemical properties of bis(trifluoromethanesulfonyl) imide intercalated graphite with first-principles calculations

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Table S1. In-plane lattice constant (a), interlayer distance (d_i) and unit cell volume of graphie obtained with PBE, and PBE + vdW functionals.

	a (Å)		d_i (Å)		Volume (Å^3)	
	Value	Error (%)	Value	Error (%)	Value	Error (%)
PBE	2.4655	0.18	3.936	17.37	41.464	18.66
vdW-DF	2.4669	0.24	3.473	3.57	36.630	4.82
vdW-DF2	2.4720	0.45	3.408	1.64	36.104	3.32
vdW-DF-obk8	2.4630	0.08	3.259	−2.82	34.262	−1.95
vdW-DF-ob86	2.4633	0.10	3.227	−3.76	33.938	−2.88
vdW-DF2-b86r	2.4635	0.10	3.225	−3.83	33.917	−2.94
vdW-DF-cx	2.4627	0.07	3.194	−4.75	33.573	−3.92
vdW-DF2-c09	2.4628	0.07	3.181	−5.13	33.441	−4.30
vdW-DF-c09	2.4623	0.05	3.153	−5.98	33.128	−5.30
DFT-D	2.4600	−0.04	3.138	−6.40	32.917	−5.80
Exp	2.461		3.353		34.944	

Table S2. Löwdin charges of atoms in graphite, isolated TFSI molecule, and TFSI-C_n compounds, where graphene means the graphene layer, and C_{face} the carbon atoms facing the O and N atoms of TFSI.

	Graphite	TFSI	TFSI-C_n				
			18	24	32	40	50
Graphene	3.962		3.902	3.915	3.925	3.931	3.936
C_{face}			3.894	3.895	3.898	3.898	3.900
TFSI		5.973	6.037	6.036	6.036	6.036	6.036
N		5.751	6.009	5.982	5.964	5.955	5.945
S		3.907	3.820	3.808	3.802	3.800	3.797
C		3.245	3.347	3.347	3.351	3.354	3.359
O		6.666	6.739	6.729	6.724	6.721	6.718
F		7.147	7.209	7.221	7.228	7.231	7.235

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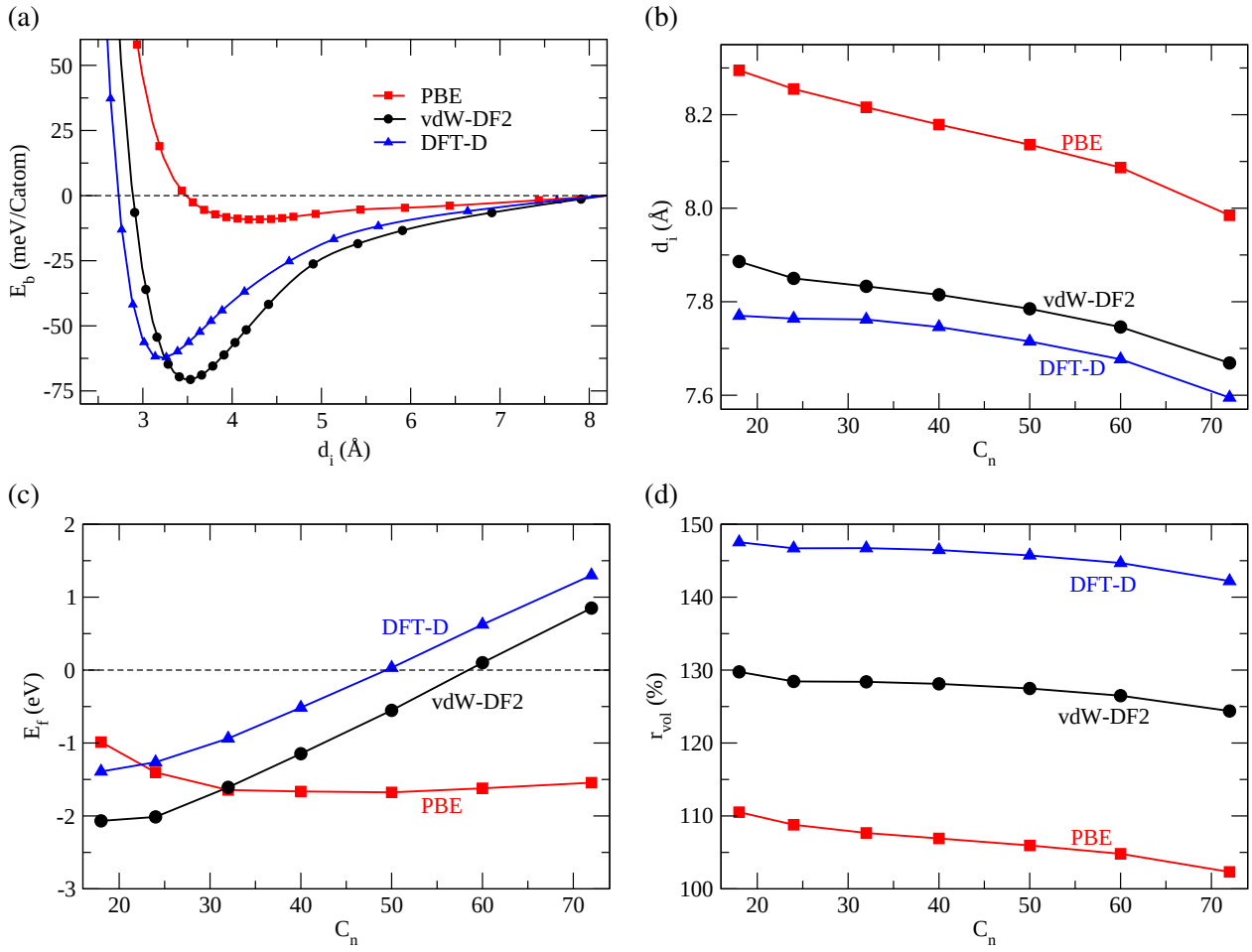

Fig. S1. (a) Interlayer binding energy in graphite, and (b) interlayer distance, (c) formation energy and (d) relative volume expansion ratio as increasing the number of carbon atoms in TFSI-C_n GICs, calculated with PBE, PBE+vdW-DF2, and PBE+DFT-D XC functionals.

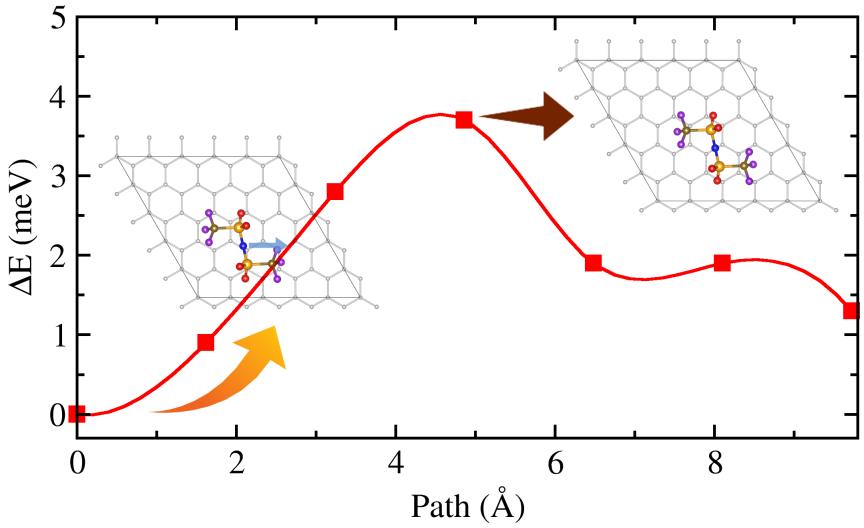

Fig. S2. Activation barrier for TFSI migration along the path indicated by blue arrow, with the starting and transition states.

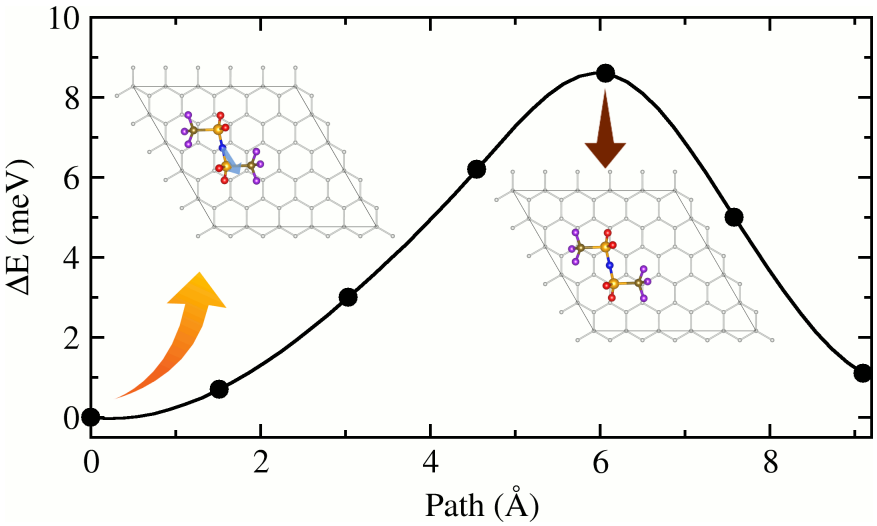

Fig. S3. Activation barrier for TFSI migration along the path indicated by blue arrow, with the starting and transition states.

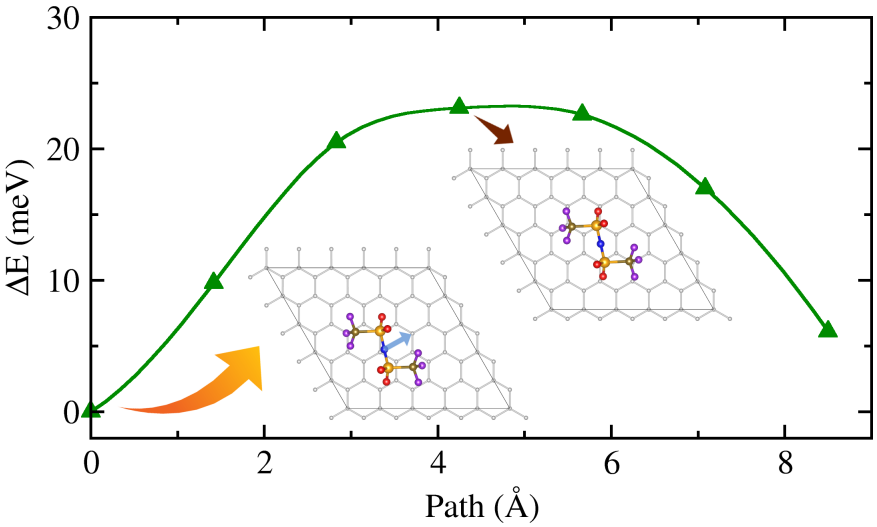

Fig. S4. Activation barrier for TFSI migration along the path indicated by blue arrow, with the starting and transition states.