Supporting Information

First-principle study on screening doped TiO_2(B) as anode material with high conductivity and low lithium transport resistance for lithium-ion batteries

Denglei Gao,[ab] Yanlei Wang,[b] Jing Kong,[b] Feng Huo,[b] Sufan Wang,*[a] Hongyan He*[b] and Suojiang Zhang [b]

[a.] *College of Chemistry and Material Science, The Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, Anhui Normal University, Wuhu 241000, PR China. E-mail: sfwang@mail.ahnu.edu.cn*

[b.] *Beijing Key Laboratory of Ionic Liquids Clean Process, CAS Key Laboratory of Green Process and Engineering, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, PR China. E-mail: hyhe@ipe.ac.cn*

Tab. S1 Experimental and calculated (GGA and GGA+*U*) structural lattice parameters of TiO_2(B).

Parameter	Literature [1]	GGA	GGA+*U*
a (Å)	12.1787	12.3030	12.5042
b (Å)	3.7412	3.7849	3.8918
c (Å)	6.5249	6.6256	6.6304
V (Å^3)	284.22	295.16	308.45
Density (g/cm^3)	3.733	3.595	3.440

Tab. S2 The four inequalities of O_v form the formation energy E_{form}, Bader charge, average bond length and band gap.

Structure	Formation energy (eV)		Bader	Average	Band
	E_{form}(Ti-rich)	E_{form}(O-rich)	Charge/e	bond length/Å	gap/eV
$O_{v\text{-}br}$	0.64	5.02	-0.91	1.84	2.55
$O_{v\text{-}3f1}$	0.29	4.68	-1.04	1.96	2.13
$O_{v\text{-}3f2}$	0.62	5.01	-1.01	1.94	2.25
$O_{v\text{-}4f}$	0.50	4.89	-1.09	2.00	1.77

Tab. S3 The lattice parameters of pure and different dopants in TiO_2(B) using GGA method.

Structure	Lattice constants(Å)			Volume	Δ*V*
	a	b	c	(Å^3)	(%)
Pure	12.3262	7.5614	13.2609	1182.33	-
N-doped	12.3295	7.5818	13.2336	1184.08	0.15
P-doped	12.3457	7.7082	13.1023	1193.09	0.91
As-doped	12.2695	7.6408	13.3193	1197.48	1.28
F-doped	12.2996	7.5865	13.2855	1186.66	0.37
Cl-doped	12.2432	7.6402	13.3579	1197.20	1.26
Br-doped	12.2320	7.6530	13.3796	1199.78	1.48
S-doped	12.2899	7.6266	13.3090	1194.91	1.06
Se-doped	12.2657	7.6460	13.3438	1199.24	1.43
Te-doped	12.2294	7.6819	13.3509	1201.59	1.63

Tab. S4 The lattice parameters of pure and different dopants in TiO_2(B) using the GGA+*U* method.

Structure	Lattice constants(Å)			Volume	Δ*V*
	a	b	c	(Å^3)	(%)
Pure	12.5151	7.7777	13.2588	1234.36	-
N-doped	12.5112	7.7929	13.2702	1236.90	0.21
P-doped	12.4985	7.8373	13.3259	1250.36	1.30
As-doped	12.5046	7.8579	13.3247	1254.48	1.63
F-doped	12.5135	7.7936	13.2922	1239.78	0.44
Cl-doped	12.5287	7.8320	13.3315	1252.01	1.43
Br-doped	12.5211	7.8345	13.3774	1255.92	1.75
S-doped	12.4951	7.8416	13.3098	1248.40	1.14
Se-doped	12.4933	7.8630	13.3391	1254.67	1.65
Te-doped	12.4705	7.8900	13.3608	1258.21	1.93

Tab. S5 The effective mass of pure and different dopants in TiO_2(B).

Structure	Effective mass (m_0) Electrons				Effective mass (m_0) Holes			
	G→F	F→Q	Q→Z	Z→G	G→F	F→Q	Q→Z	Z→G
Pure	1.016	1.883	**0.672**	1.359	1.318	0.895	8.682	**0.808**
N-doped	1.156	2.626	**0.631**	2.082	3.293	**1.060**	4.250	1.508
P-doped	0.485	18.678	**0.393**	10.408	1.668	**1.201**	4.638	2.922
As-doped	0.516	24.155	**0.506**	11.463	1.568	**1.260**	5.052	3.319
F-doped	**0.504**	4.111	0.682	3.737	1.871	**0.938**	1.950	1.372
Cl-doped	2.605	7.759	**1.419**	4.876	1.637	**1.185**	1.288	3.324
Br-doped	**0.844**	11.843	0.853	19.833	3.770	**2.188**	3.857	5.213
S-doped	0.674	6.168	**0.478**	4.985	1.718	1.962	**1.120**	5.181
Se-doped	0.851	7.195	**0.418**	17.295	6.737	1.160	**0.385**	4.879
Te-doped	**0.982**	37.481	3.337	8.224	4.533	**1.941**	9.582	12.171

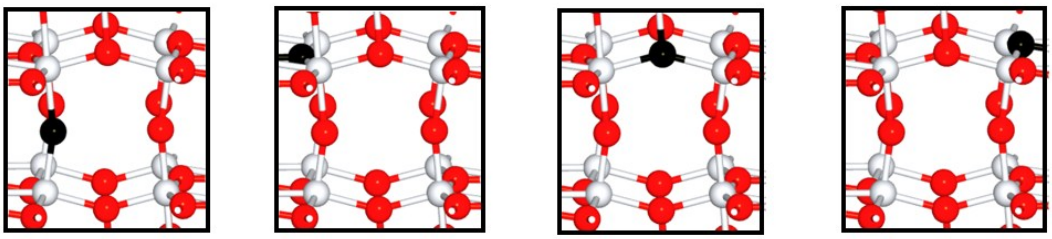

Fig. S1 Various oxygen vacancies are enriched in the *b*-axis channel direction.

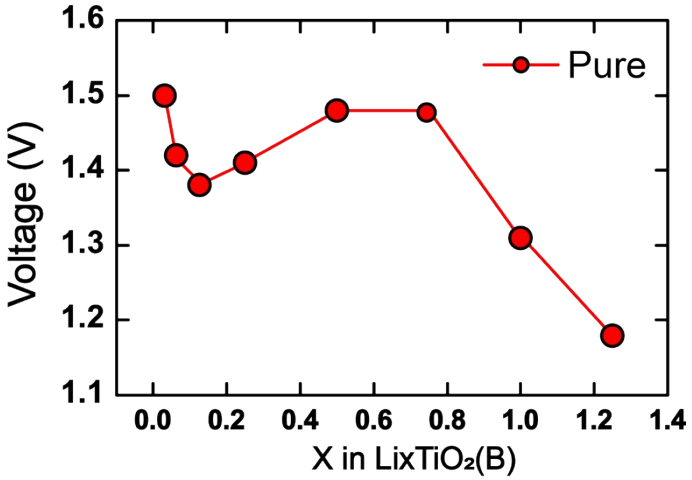

Fig. S2 The average equilibrium voltage of TiO_2(B) in the lithiated state from low to high concentration was calculated using GGA+*U* method.

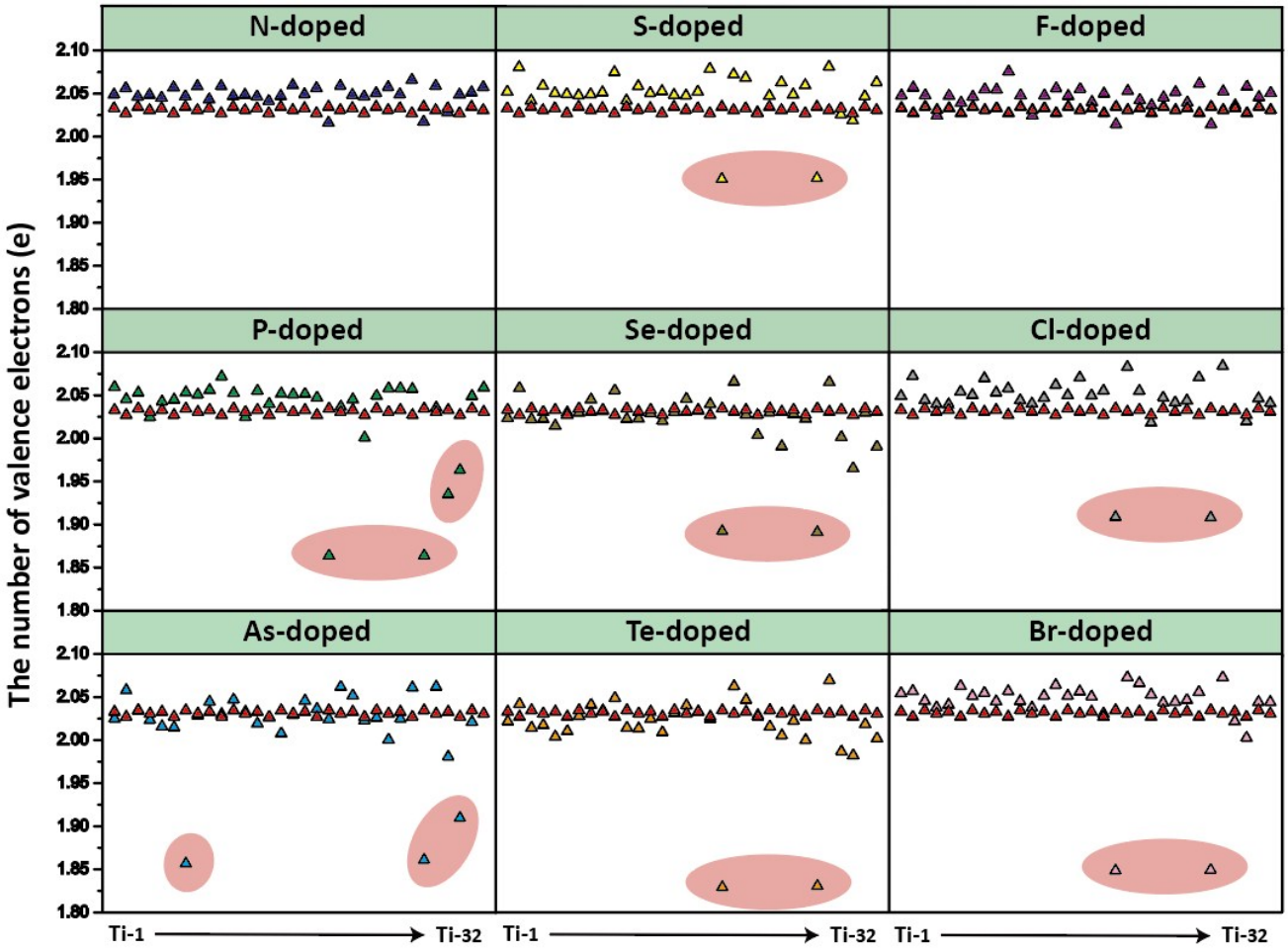

Fig. S3 The Bader charge of Ti atom for pure and doped TiO_2(B), and the red triangle represents the pure TiO_2(B).

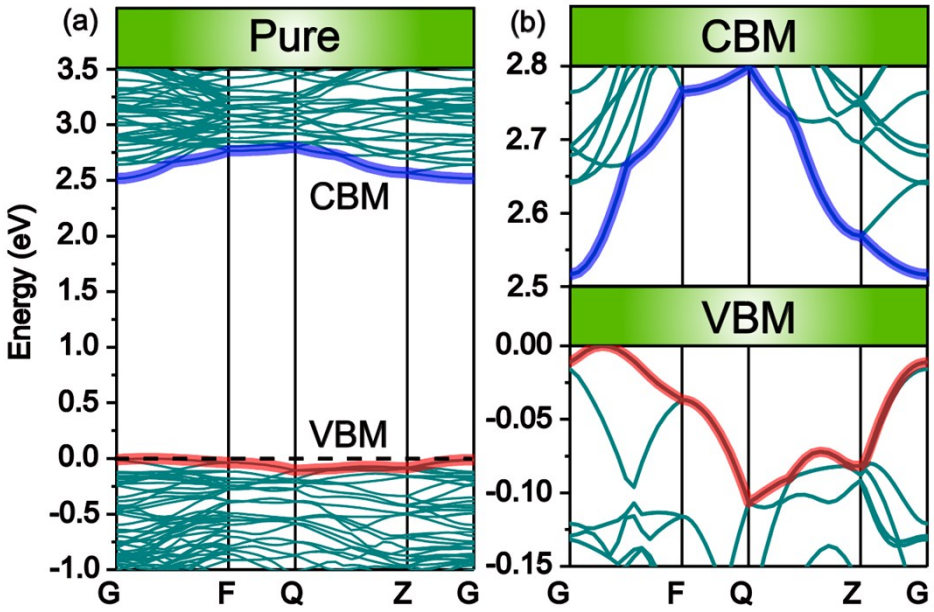

Fig. S4 (a) Band structures of pure TiO_2(B). The dark cyan lines represent the contribution of the entire system. The bands projected to CBM and VBM are highlighted by blue and red lines.The horizontal black dashed lines indicate the E_F. (b) Contributions of CBM and VBM.

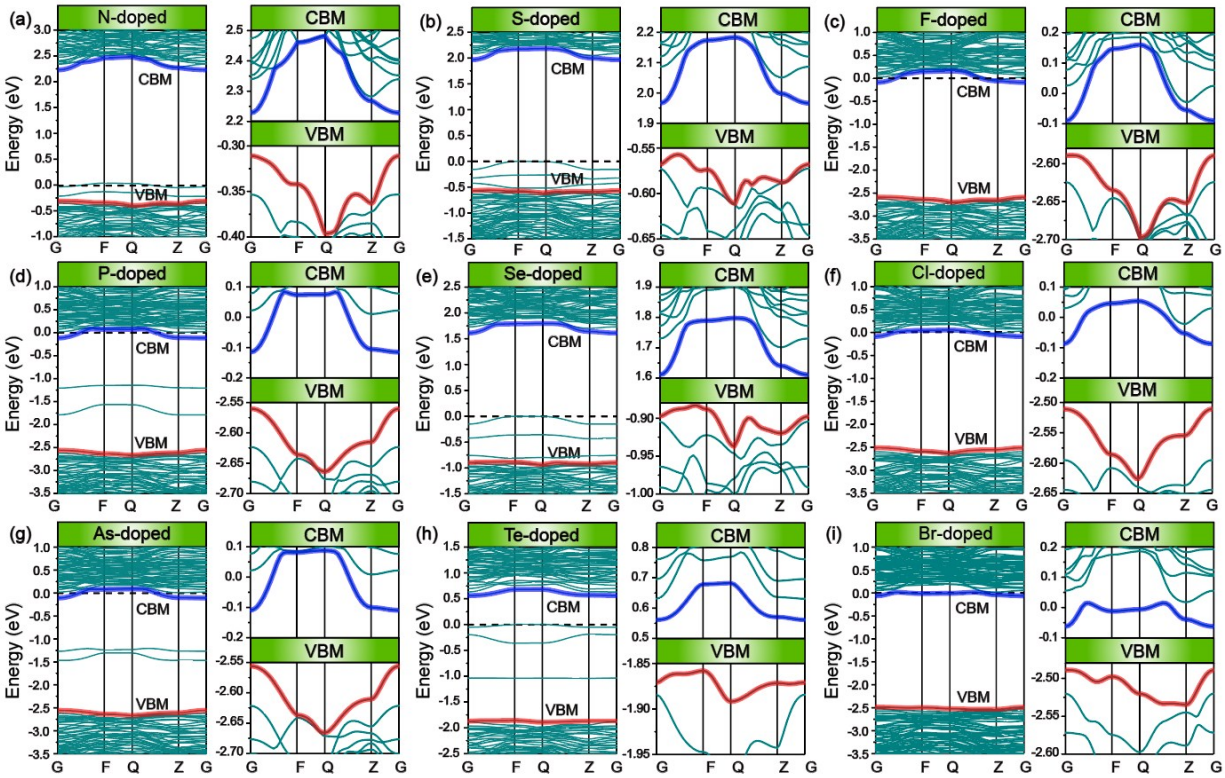

Fig. S5 (a-i) Band structures of different dopants in TiO_2(B). The dark cyan lines represent the contribution of the entire system. The bands projected to CBM and VBM are highlighted by blue and red lines. The horizontal black dashed lines indicate the E_F.

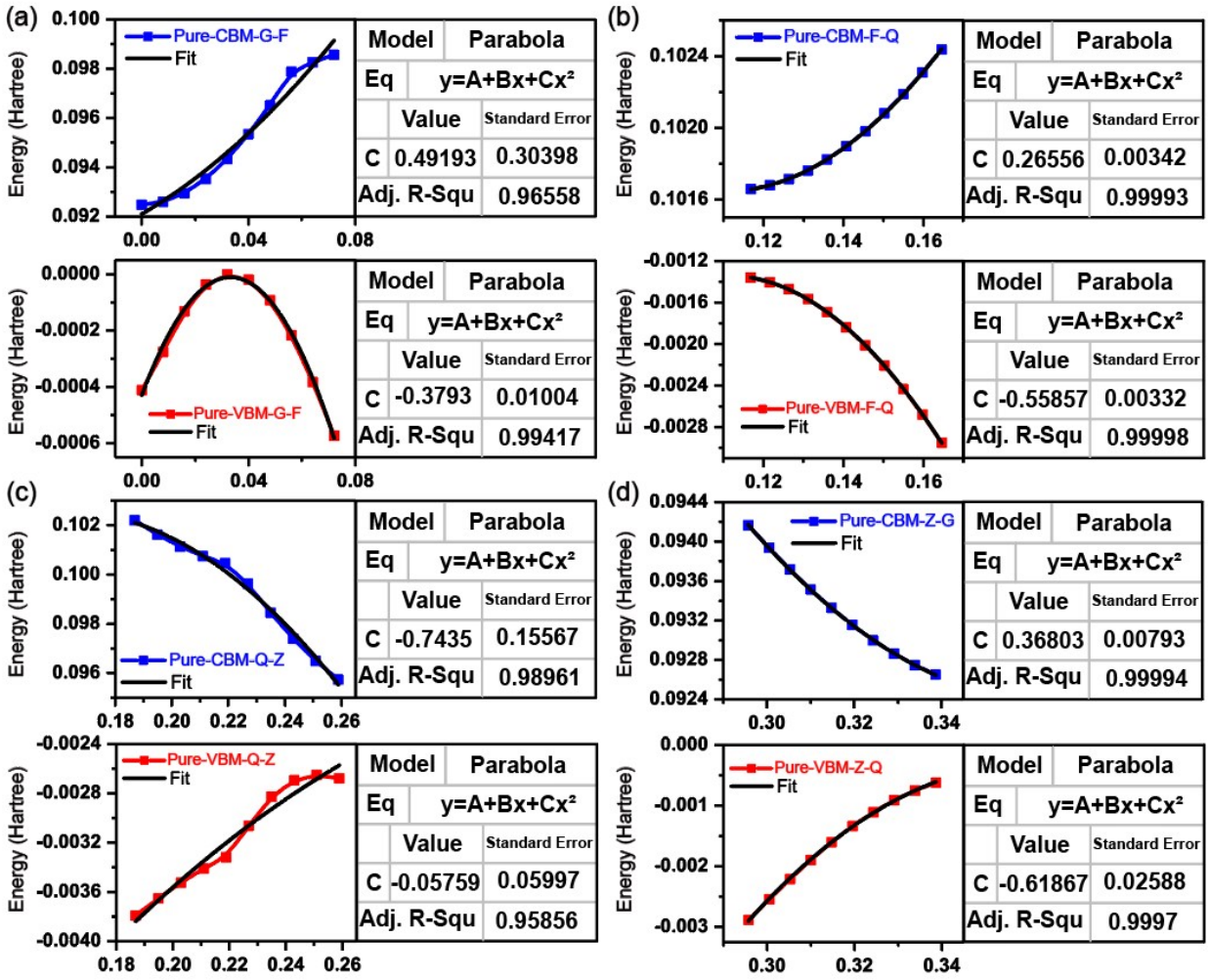

Fig. S6 The CBM and VBM curves along the (a) G-F, (b) F-Q, (c) Q-Z and (d) Z-G direction in TiO_2(B). Black solid lines are the fitting curves. The table shows the fitting method, the quadratic C value and the standard error.

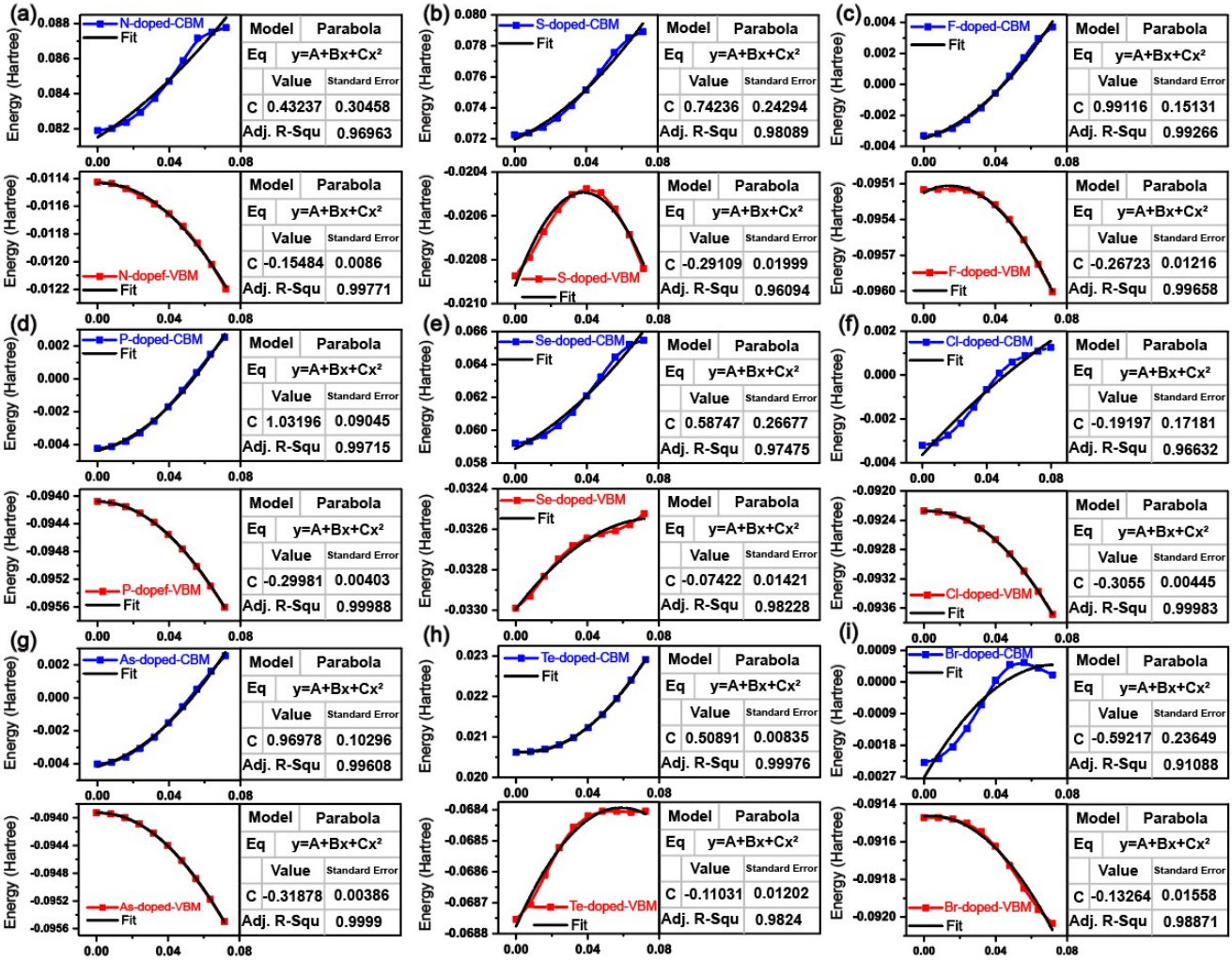

Fig. S7 (a-i) The CBM and VBM curves along the G-F direction in different dopants TiO_2(B). Black solid lines are the fitting curves. The table shows the fitting method, the quadratic C value and the standard error.

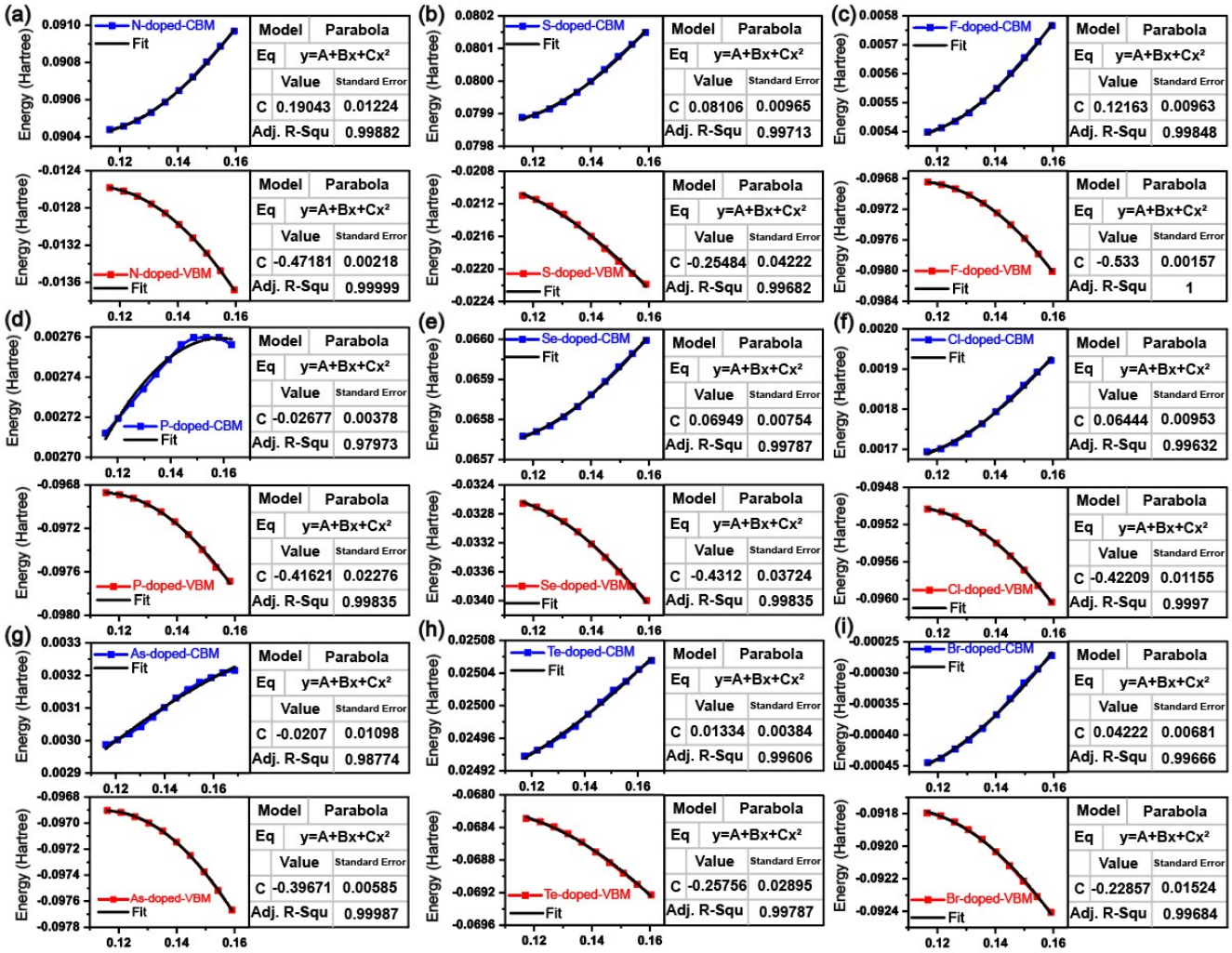

Fig. S8 (a-i) The CBM and VBM curves along the F-Q direction in different dopants TiO_2(B). Black solid lines are the fitting curves. The table shows the fitting method, the quadratic C value and the standard error.

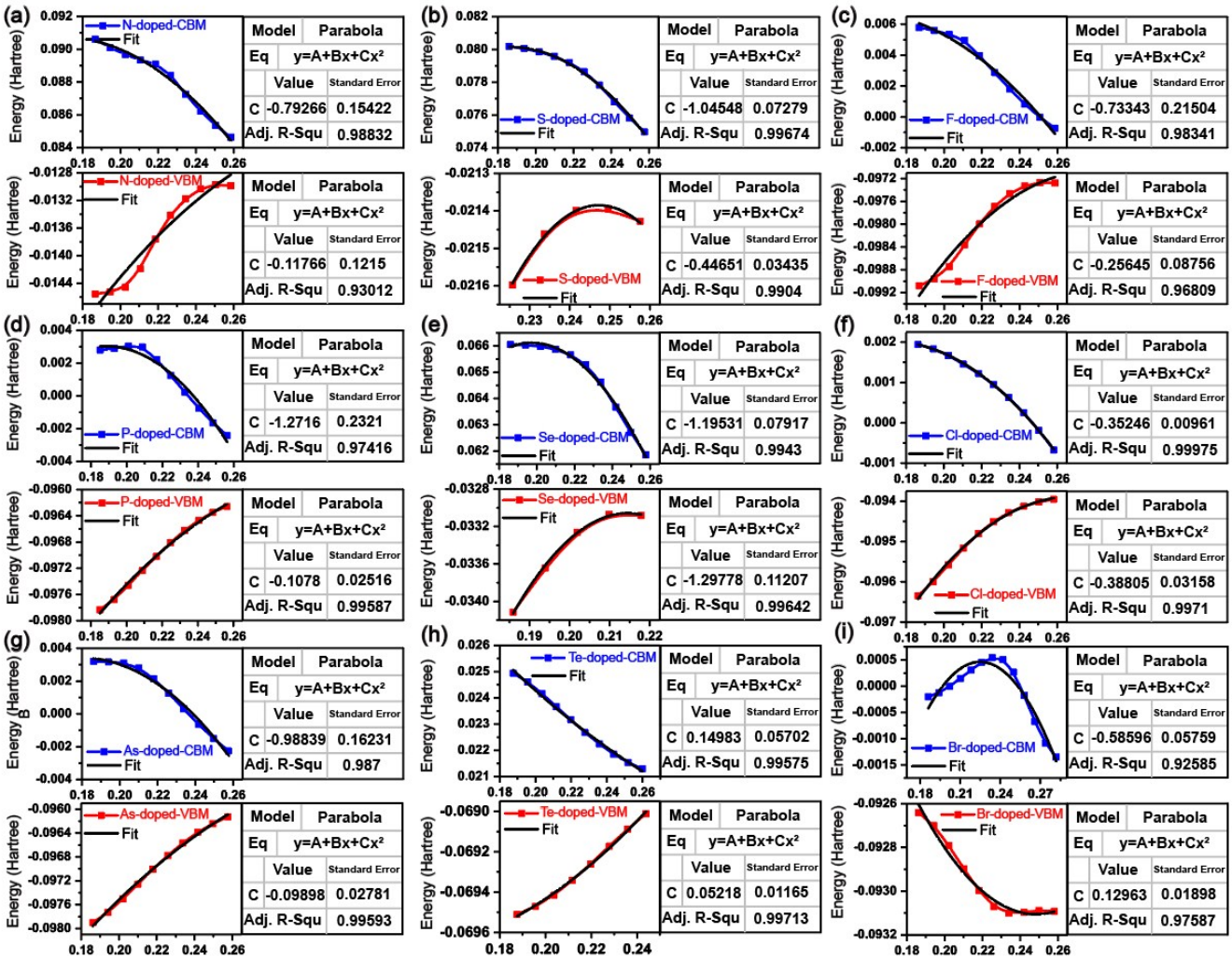

Fig. S9 (a-i) The CBM and VBM curves along the Q-Z direction in different dopants TiO_2(B). Black solid lines are the fitting curves. The table shows the fitting method, the quadratic C value and the standard error.

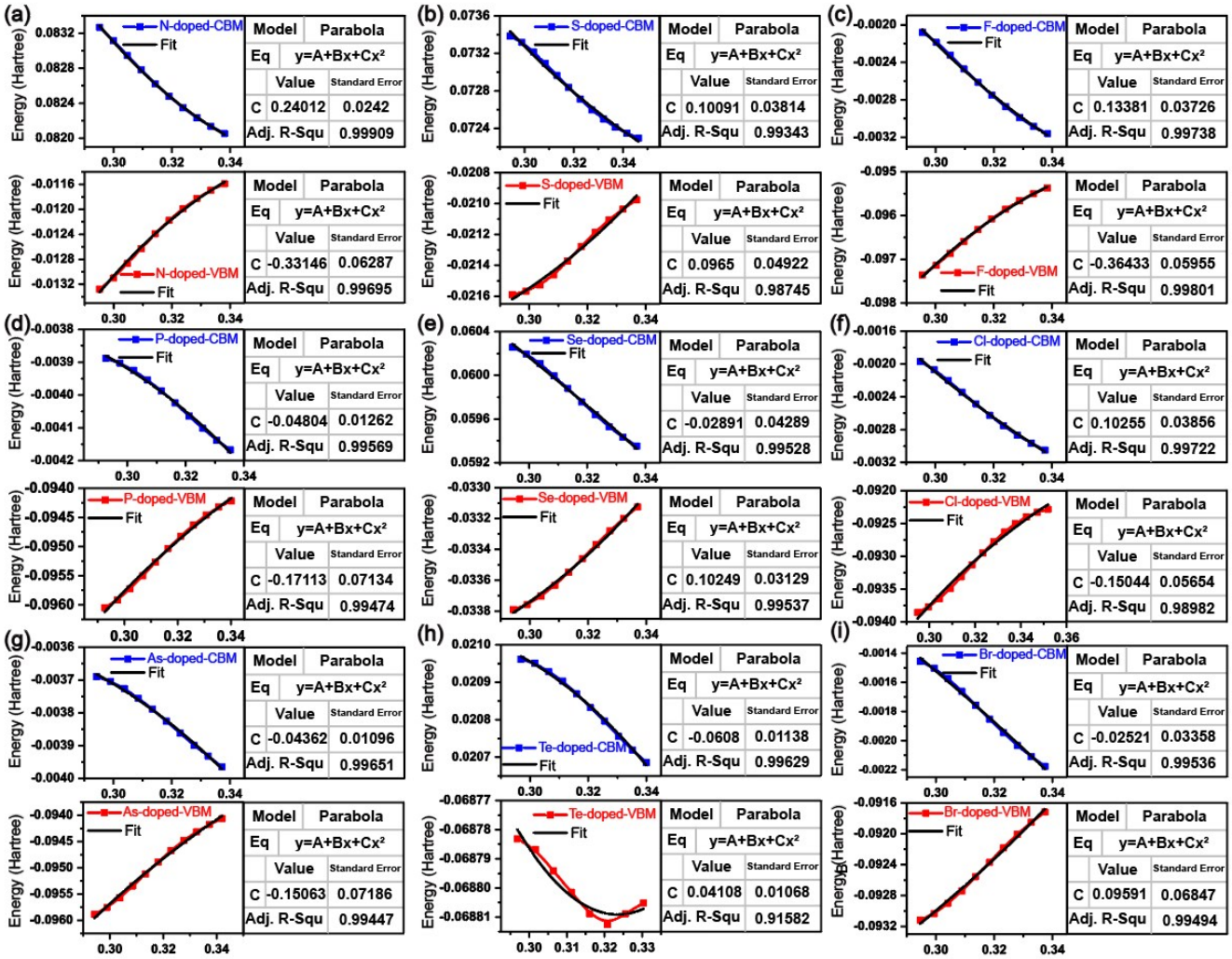

Fig. S10 (a-i) The CBM and VBM curves along the Z-G direction in different dopants TiO_2(B). Black solid lines are the fitting curves. The table shows the fitting method, the quadratic C value and the standard error.

Supplementary References

1 C. Arrouvel, S. C. Parker and M. S. Islam, *Chem. Mater.*, 2009, **21**, 4778-4783.