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

Two-Dimensional Dirac TiB_2C_2 as a Potential Anode Materials for Li-Ion Batteries: A First-Principles Study

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Table S1: Convergence test for cutoff energy of plane wave.

Cutoff energy (eV) (Ry)	Total energy /atom (eV/atom)	Absolute error (meV)
340.14259941 (25)	-662.1342917	- - -
408.17111929 (30)	-662.8512307	716.939
476.19963917(35)	-663.0572755	206.0448
544.22815905 (40)	-663.1146371	57.3616
612.25667893 (45)	-663.1303925	15.7554
748.3137187 (55)	-663.1389369	8.5444
816.34223858 (60)	-663.1414404	2.5035
884.37075846 (65)	-663.1433825	1.9421
952.39927834 (70)	-663.1448193	1.4368
1020.4277982 (75)	-663.1458342	1.0149
1088.4563181 (80)	-663.146447	0.6128

Table S2: Convergence test for K-point mesh.

K-point meshes [K×K×1]	Total energy /atom (eV/atom)	Absolute error (meV)
[6×6×1]	-663.1335077	- - -
[9×9×1]	-663.1299739	3.5338
[12×12×1]	-663.1391506	9.1767
[15×15×1]	-663.1303496	8.801
[18×18×1]	-663.1305766	2.2706
[21×21×1]	-663.1303651	2.1156
[24×24×1]	-663.1303657	0.0006

Table S3: Adsorption energy without and with dipole correction

Adsorption sites	H_{Ti}**-site**	T_C**-site**	T_B**-site**
Without Dipole correction			
Adsorption Energy (eV)	- 1.6320450091	- 1.0892374216	- 0.9292924392
With Dipole correction			
Adsorption Energy (eV)	-1.5845681867	- 1.0119151113	- 0.8516292475

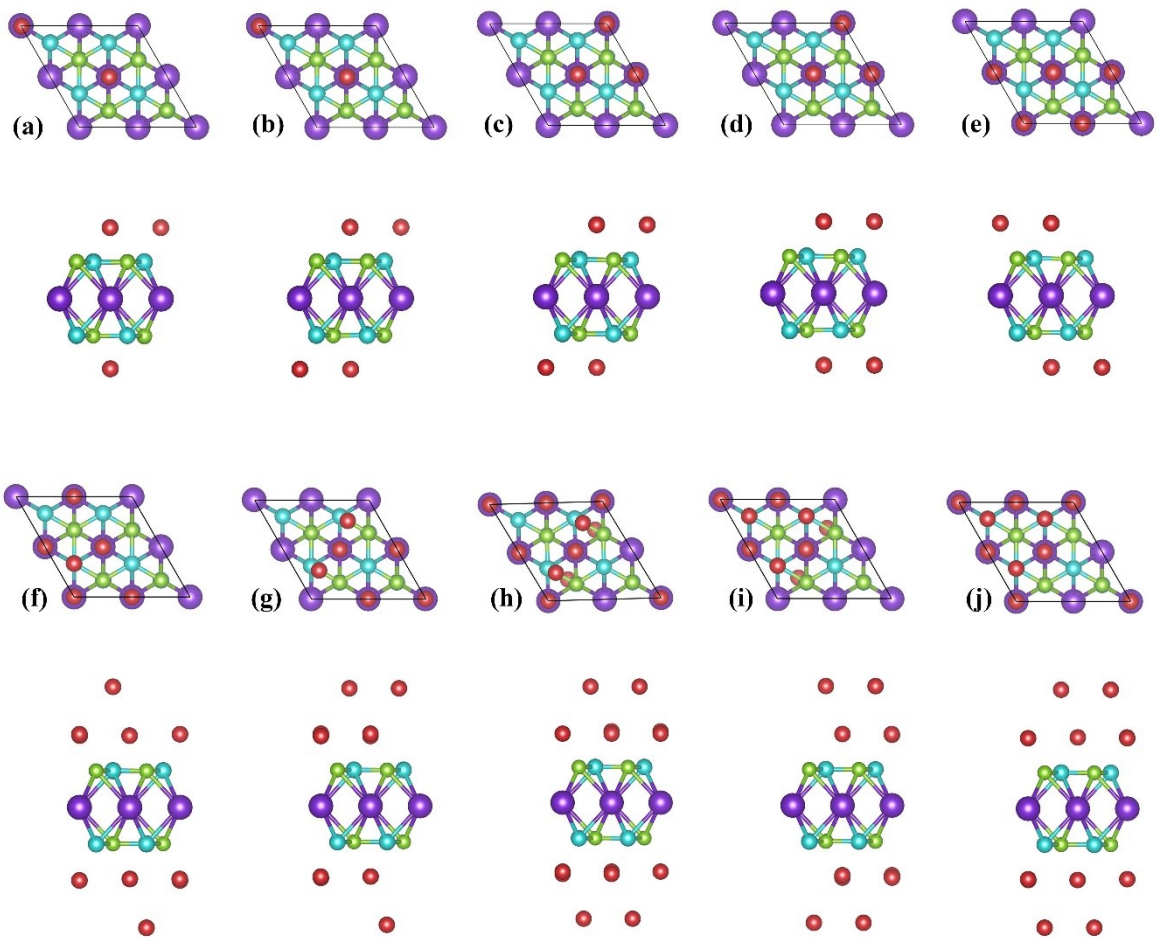

Figure S1: Top and side view of metastable structures with different Li concentrations in the TiB_2C_2 monolayer. (a) $Li_{0.75}TiB_2C_2$; (b) $Li_1TiB_2C_2$; (c) $Li_{1.25}TiB_2C_2$; (d) $Li_{1.5}TiB_2C_2$; (e) $Li_{1.75}TiB_2C_2$; (f) $Li_{2.5}TiB_2C_2$; (g) $Li_{2.75}TiB_2C_2$; (h) $Li_3TiB_2C_2$; (i) $Li_{3.25}TiB_2C_2$ and (j) $Li_{3.5}TiB_2C_2$.