Supplementary Information

Functionalized Two-Dimensional Iron Boride Compounds as a Novel Electrode Material in Li-Ion Batteries

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Table S1 shows the calculated elastic constant Cij for 2D FeB

System	C_{11}(N/m)	C_{12}(N/m)	C_{66}(N/m)
FeB	192.775	24.778	91.866

Two-dimensional crystals differ from three-dimensional materials in that there is zero stress outside the two-dimensional plane. As a result, the elastic coefficient matrix of a two-dimensional crystal has reduced dimensionality, which can be expressed using the following formula:

$$c = \begin{bmatrix} c_{11} & c_{12} & c_{16} \\ c_{12} & c_{22} & c_{26} \\ c_{16} & c_{26} & c_{66} \end{bmatrix}$$

Based on the energy-strain relationship, the elastic constants of FeB are calculated as C_{11}=192.775 N/m, C_{12}=24.778 N/m, and C_{66}=91.866 N/m. The stability criteria of $C_{11} > C_{12}$ and $C_{66} > 0$ are satisfied, indicating that the two-dimensional FeB is mechanically stable.

Table S2 The energy of four different adsorption configurations of functional groups (F, O and S) on FeB surface.

Configurations	S1(eV)	S2(eV)	S3(eV)	S4(eV)
FeBF	-344.445	-334.312	-344.939	-344.785
FeBO	-368.909	-356.046	-377.796	-374.044
FeBS	-353.326	-344.456	-353.045	-359.072

Table S3 The bond length and layer thickness parameters of the most stable configuration of functionalized FeBT (T = F, O and S).

Configurations	$L_{(B-B)}$ (Å)	$L_{(Fe-B)}$ (Å)	Thickness(Å)
FeBF	1.682	2.174	2.748
FeBO	1.657	2.231	2.951
FeBS	1.702	2.092	2.361

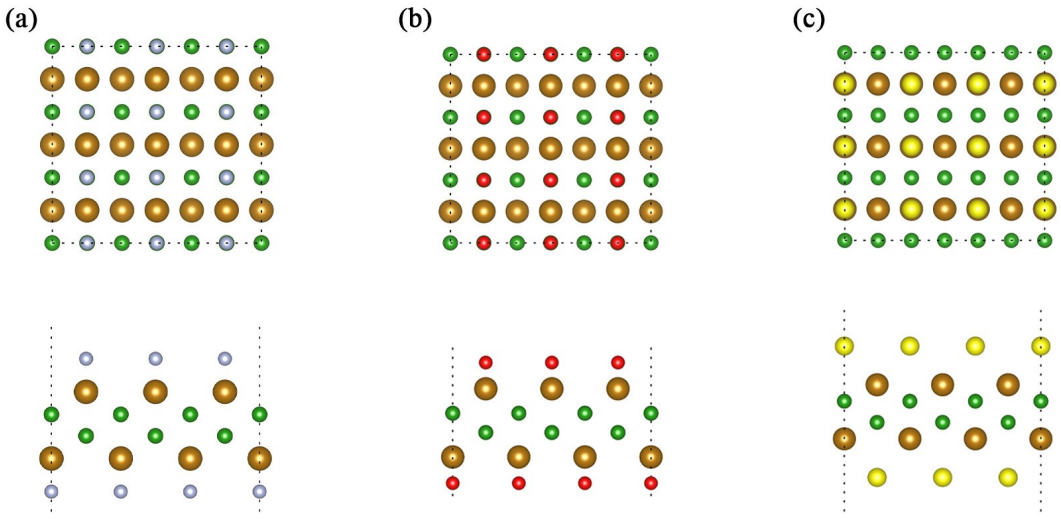

Fig. 2 Top and front views of the most stable configurations for functionalized FeBT (T = F, O, and S) are shown.

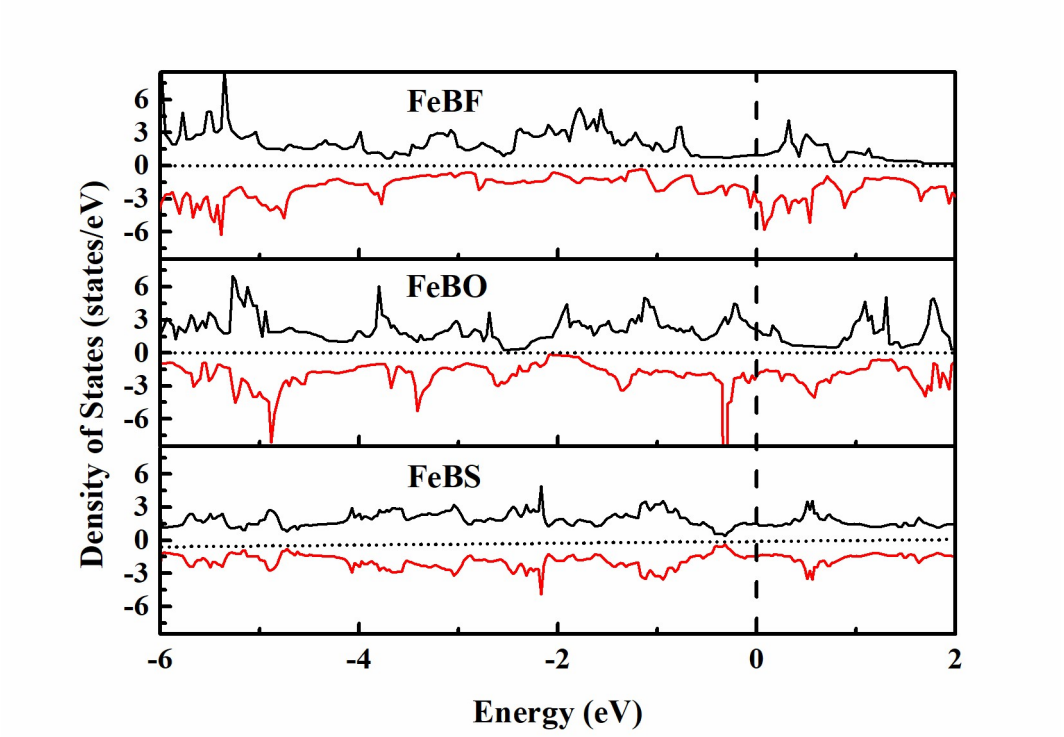

Fig. 3 DOS for functionalized FeBT (T = O, F, and S) are shown with the Fermi energy set to 0 eV, indicated by the vertical dashed line.

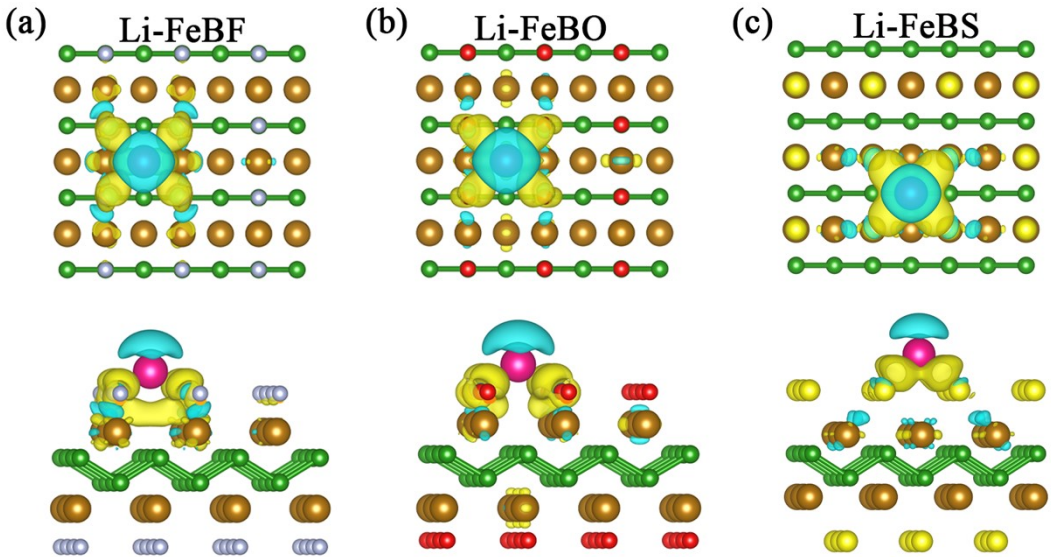

Fig. 4 The charge density differences of FeBT (T = O, F, and S) were calculated upon the adsorption of a single Li atom. Getting electrons and losing electrons were represented by the pale yellow and blue areas.

Table S4 The calculated energy for FeB at four adsorption sites of Li atoms after considering zero-point vibrational energy.

Whether to consider the zero-point energy correction	S1(eV)	S2(eV)	S3(eV)	S4(eV)
No	-266.69994	-267.09992	-266.83135	-266.85917
Yes	-266.67577	-267.05499	-266.78682	-266.82693
Zero-point energy	0.024174	0.044934	0.044531	0.032242

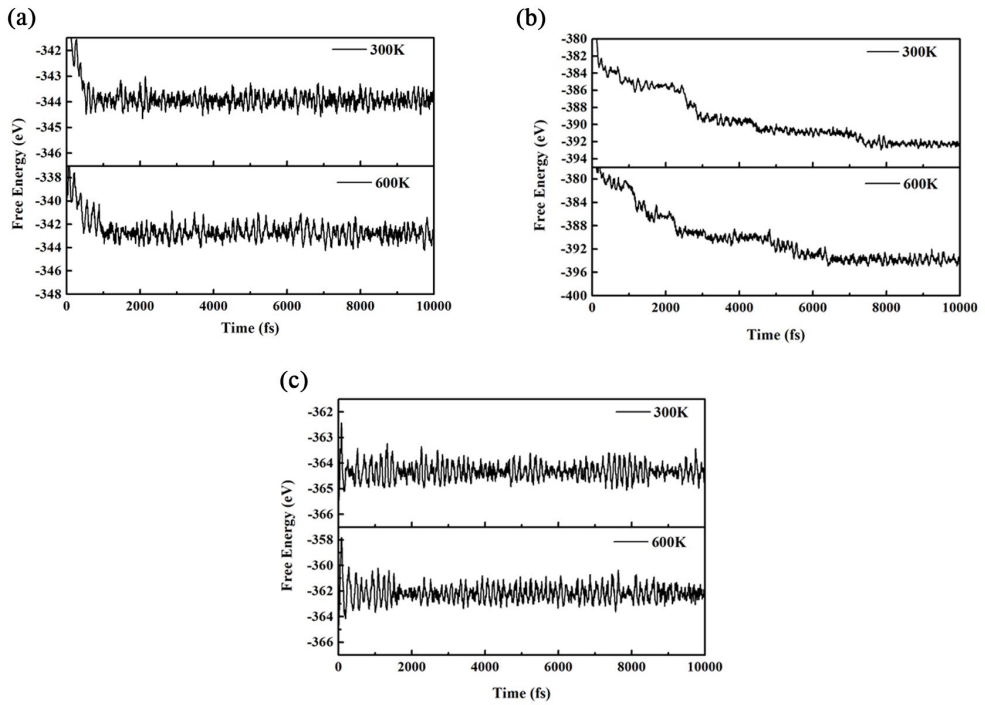

Fig. 5 The Molecular dynamics simulations of (a) FeBF, (b) FeBO, and (c) FeBS were conducted at 300K and 600K.