Mo_2B, a MBene member with high electrical and thermal conductivities, and satisfactory performances in lithium ion batteries

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The specific heat is calculated according to the following equation:

$$c = \frac{1}{N_k M}\sum_{s,k} k_B \left(\frac{\hbar\omega_{s,k}}{k_B T}\right)^2 \frac{\exp\left(\hbar\omega_{s,k}/k_B T\right)}{\left[\exp\left(\hbar\omega_{s,k}/k_B T\right)-1\right]^2} \backslash *$$

MERGEFORMAT (S1),

Here, N_k and M denote the number of k-points adopted, and the mass of the Mo_2B unitcell, respectively. k_B and $\hbar$ are the Boltzmann's and the reduced Plank's constants, respectively. T represents temperature. $\omega_{s,k}$ is the circular phonon frequency of s branch at k point.

The thermal expansion coefficient is calculated according to the Grüneisen approximation. The detailed equation is as follows:

$$\alpha = \frac{1}{\mathrm{N_k}} \frac{1}{\mathrm{a_0^2}\frac{\partial^2 \mathrm{E}}{\partial \mathrm{a}^2}\Big|_0} \sum_{\mathrm{s,k}} \mathrm{c(s,k)}\gamma(\mathrm{s,k}) \backslash * \quad \text{MERGEFORMAT}$$

(S2),

where a_0 is the optimal lattice parameter, E denotes the total energy of the configuration investigated. $\gamma(s,k)$ represents the Grüneisen parameter, which is calculated as $\gamma(s,k) = \frac{-a_0}{\omega_{0,s,k}} \frac{\partial \omega_{s,k}}{\partial a}$.

The phonon thermal conductivity is calculated according to the Klemens's theory:

$$\kappa_p = \frac{\rho}{T}\sum_s \frac{<\upsilon_s>^4}{<\gamma_s^2>} \frac{1}{\omega_{\max,s}} \ln\frac{\omega_{\max,s}}{\omega_{\min,s}} \backslash * \quad \text{MERGEFORMAT}$$

(S3),

where ρ is the mass density, υ_s and γ_s are the group velocity and Grüneisen parameter of branch s. $\omega_{\max,s}$ and $\omega_{\min,s}$ are the maximum and minimum circular phonon frequency of branch s.

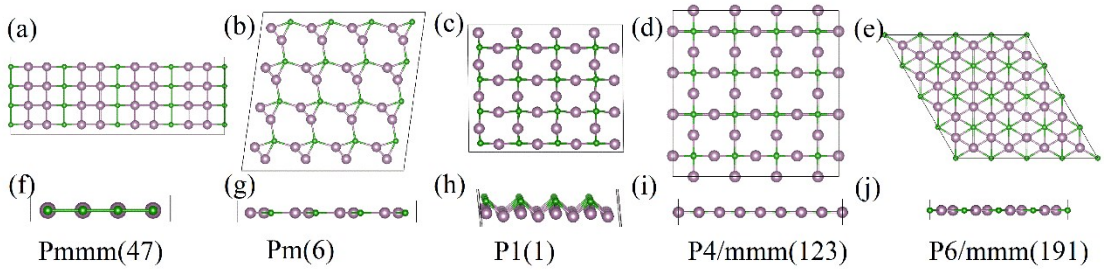

Figure S1. Some metastable two-dimensional molybdenum borides with the ratio of molybdenum to boron is 2:1, predicted from a combination of the CALYPSO and VASP codes.

Table S1. Relative total energies ΔE (in eV) between the unit cells of the metastable configurations presented in Figure S1 and the H- and T-type Mo_2B. The space group is adopted to differentiate these structures, and 187 and 164 denote the H- and T-type Mo_2B, respectively.

Space group	47	6	1	123	191	187	164
ΔE	4.91	4.20	2.51	5.17	3.59	0.0525	0.000

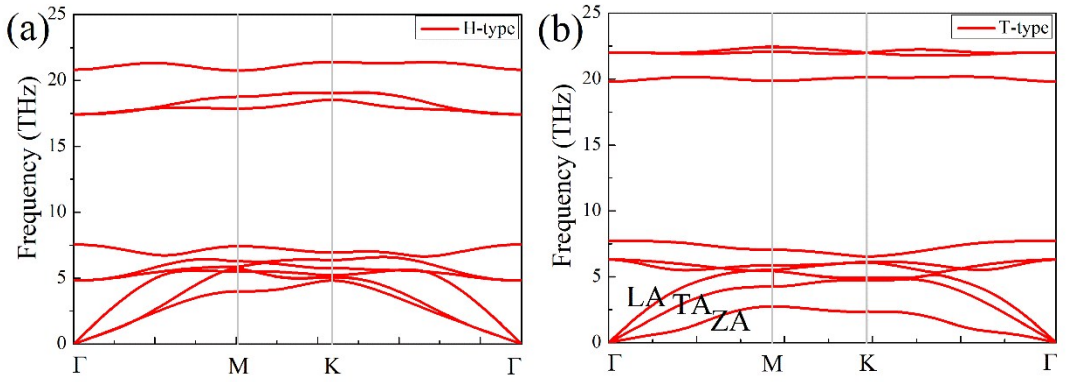

Figure S1. The phonon dispersions of the (a) H-type and (b) T-type Mo_2B.

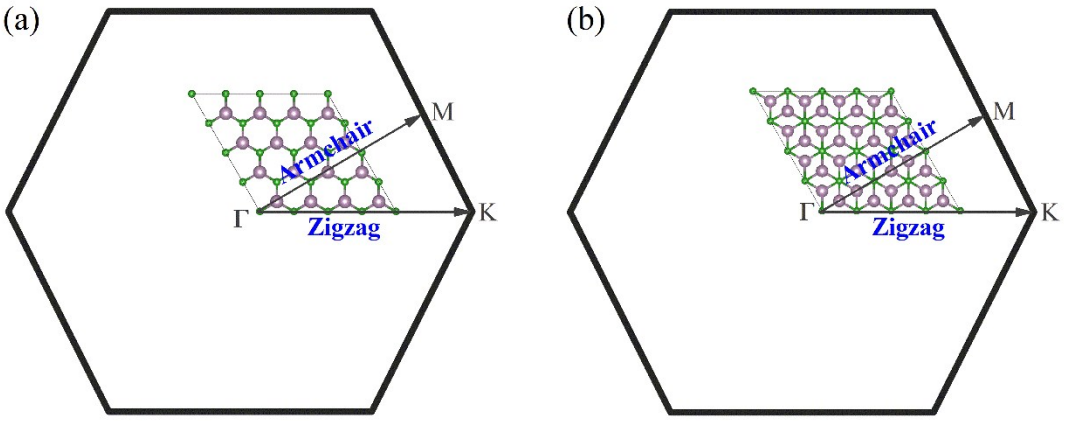

Figure S2. The Brillouin zones (BZs) for the H- and T-type Mo_2B, where the high-symmetry directions ΓM and ΓK respectively correspond to the armchair and zigzag directions in both the H- and T-type configurations.

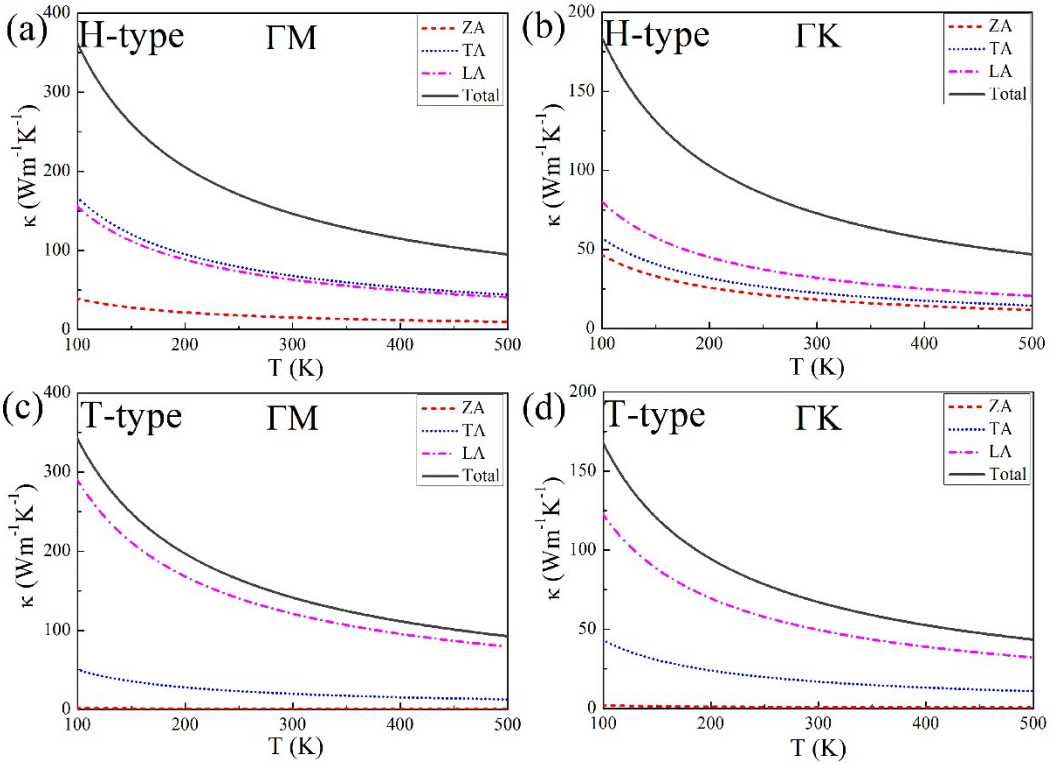

Figure S3. Based on a 5 μm flake length, (a) and (b) respectively shows the phonon thermal conductivity along the armchair (ΓM) and zigzag (ΓK) direction of the H-type Mo_2B. (c) and (d) respectively shows the corresponding value along the armchair and zigzag direction of the T-type Mo_2B.

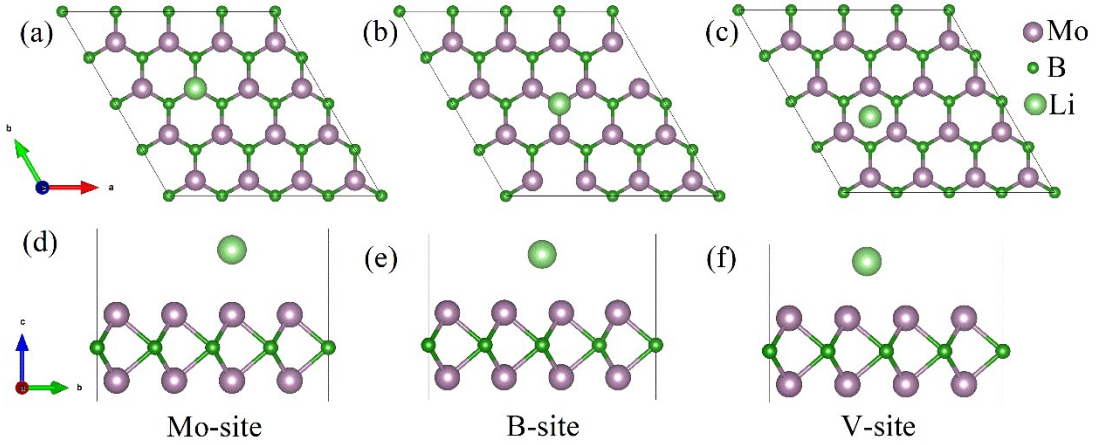

Figure S4. (a) and (d) respectively show the top-view and side-view of the H-type Mo_2B with one Li atom on the top-site of the Mo atom, and this configuration is denoted as "Mo-site"; (b) and (e) are the top-view and side-view of the H-type Mo_2B with one Li atom on the top-site of the middle boron atom, the configuration of which is denoted as "B-site". (c) and (f) respectively present the top-site and side-view of the H-type Mo_2B with one Li atom on the top-site of the hexagonal center, and the structure is represented as "V-site".

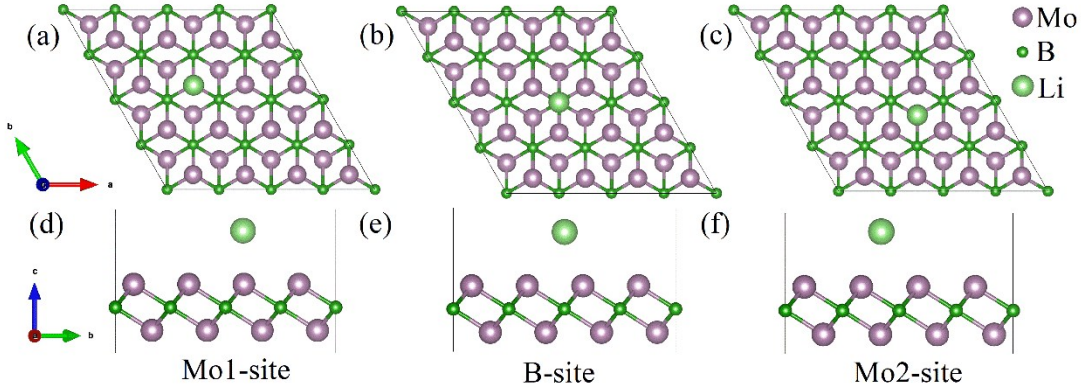

Figure S5. (a) and (d) are respectively the top-view and side-view of the T-type Mo_2B with one Li atom on the top-site of the neighboring Mo atom, and the structure is denoted as "Mo1-site"; (b) and (e) are respectively the top-view and side-view of the T-type Mo_2B with one Li atom on the top-site of the middle boron atom, which is named as "B-site"; (c) and (f) respectively shows the top-view and side-view of the T-type Mo_2B with one Li atom on the top-site of the bottom Mo atom, and this structure is denoted as "Mo2-site".

Table S2. The relative total energies (in eV) for one Li atom on different sites of both the H- and T-type Mo_2B.

H-type	Mo-site	B-site	V-site
	0.0263	0.128	0.000
T-type	Mo1-site	B-site	Mo2-site
	0.0198	0.0125	0.000

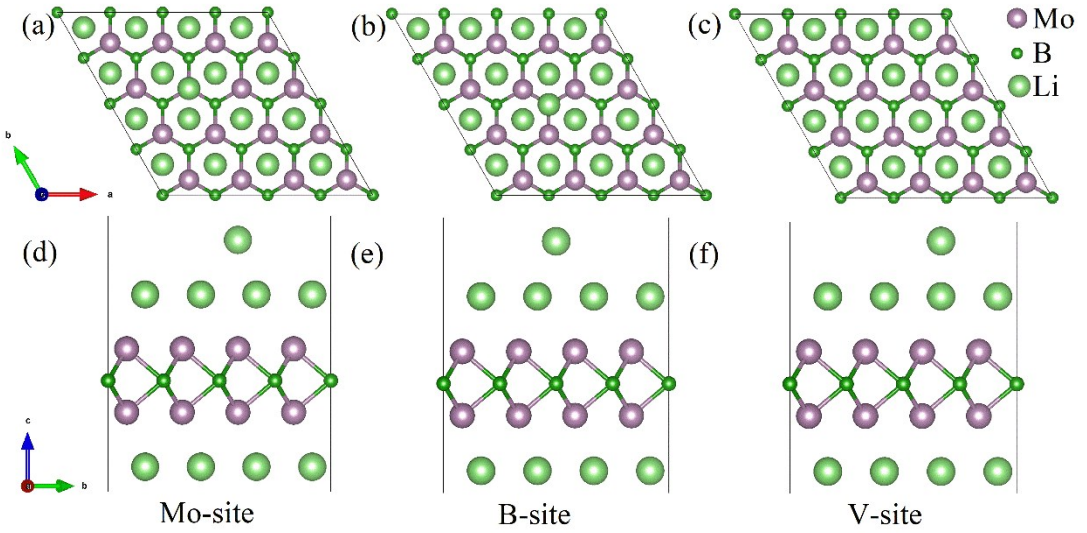

Figure S6. (a) and (d) respectively show the top-view and side-view of the H-type Mo_2B with thirty-three Li atoms, and the thirty-three Li atom is on the top-site of the Mo atom, and this configuration is denoted as "Mo-site"; (b) and (e) are the top-view and side-view of the H-type Mo_2B with thirth-three Li atoms, with the thirty-three Li atom on the top-site of the middle boron atom, and which structure is denoted as "B-site". (c) and (f) respectively present the top-site and side-view of the H-type Mo_2B with thirty-three Li atoms, and the thirty-three Li atom is on the top-site of the hexagonal center, and the structure is represented as "V-site".

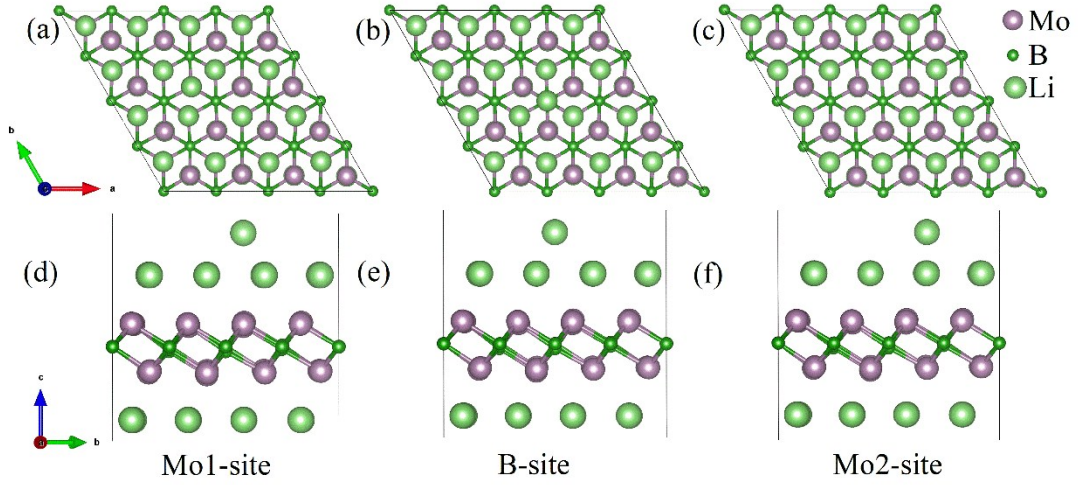

Figure S7. (a) and (d) respectively show the top-view and side-view of the T-type Mo_2B with thirty-three Li atoms, and the thirty-three Li atom is on the top-site of the top Mo atom, and this configuration is denoted as "Mo1-site"; (b) and (e) are the top-view and side-view of the T-type Mo_2B with thirty-three Li atoms, with the thirty-three Li atom on the top-site of the middle boron atom, and which structure is denoted as "B-site". (c) and (f) respectively present the top-site and side-view of the T-type Mo_2B with thirty-three Li atoms, and the thirty-three Li atom is on the top-site of the bottom Mo atom, and the structure is represented as "Mo2-site".

Table S3. The relative total energies (in eV) for the thirty-three Li atom on different sites of both

the H- and T-type Mo_2B.

H-type	Mo-site	B-site	V-site
	0.000	0.00835	0.00852
T-type	Mo1-site	B-site	Mo2-site
	0.000	0.00648	0.0326