Electronic supplementary materials

For https://doi.org/10.1631/jzus.A2400503

Electrostatic potential distribution image-transfer learning method for highly accurate prediction of lithium diffusion barriers on transition metal dichalcogenide surfaces

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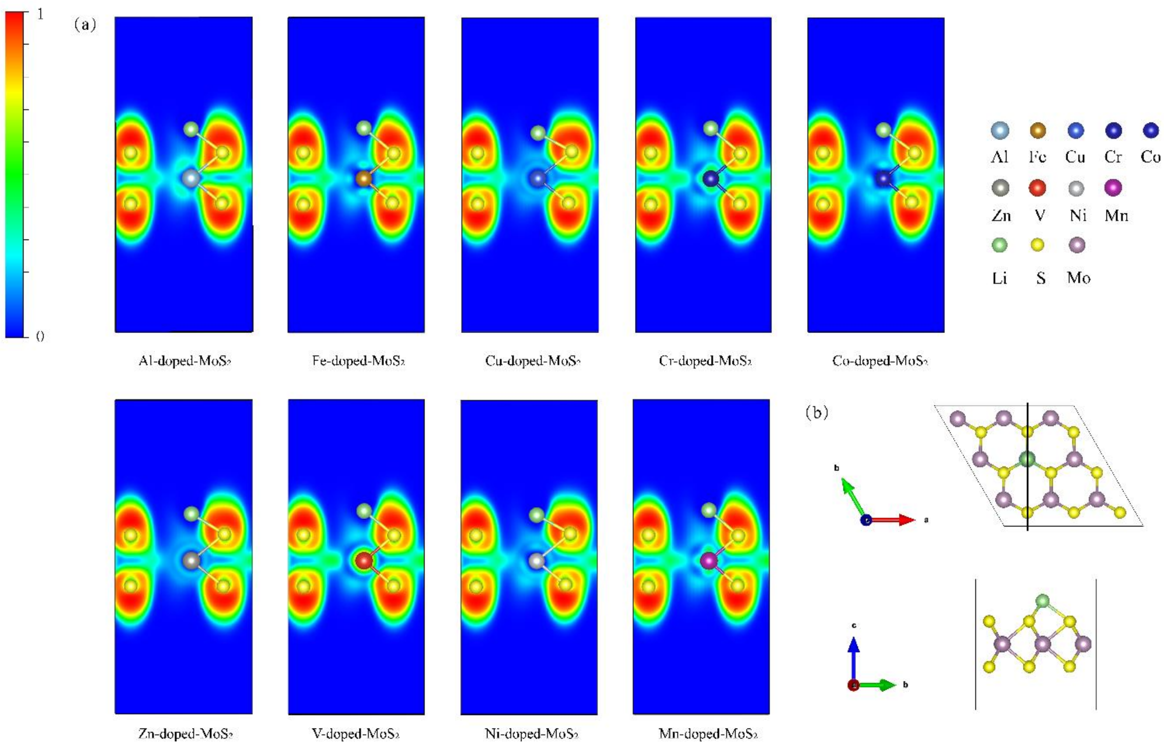

Fig. S1: (a) The ELF of Metal elements (Al, Fe, Cu, Cr, Co, Zn, V, Ni, Mn) doped MoS_2 surfaces with Li atom absorbed,(b) Schematic diagram of adsorption structure, the black line marks the plane of ELF

$$E_{barrier} = E_{system-sp} - E_{system-vp} \tag{S1}$$

$$E_{b-sp} = E_{Li} + E_{surface} - E_{system-sp} \tag{S2}$$

$$E_{b-vp} = E_{Li} + E_{surface} - E_{system-vp} \tag{S3}$$

$$E_{barrier} = E_{b-vp} - E_{b-sp} \tag{S4}$$

where $E_{barrier}$ represents the diffusion barrier, $E_{system-vp}/E_{system-sp}$ represents the system energy of Li atom located at saddle/valley point, E_{b-vp}/E_{b-sp} represents the binding energy of Li atom located at saddle/valley point, E_{Li} represents the energy of single Li atom, and $E_{surface}$ represents the energy of metal element doped surface.

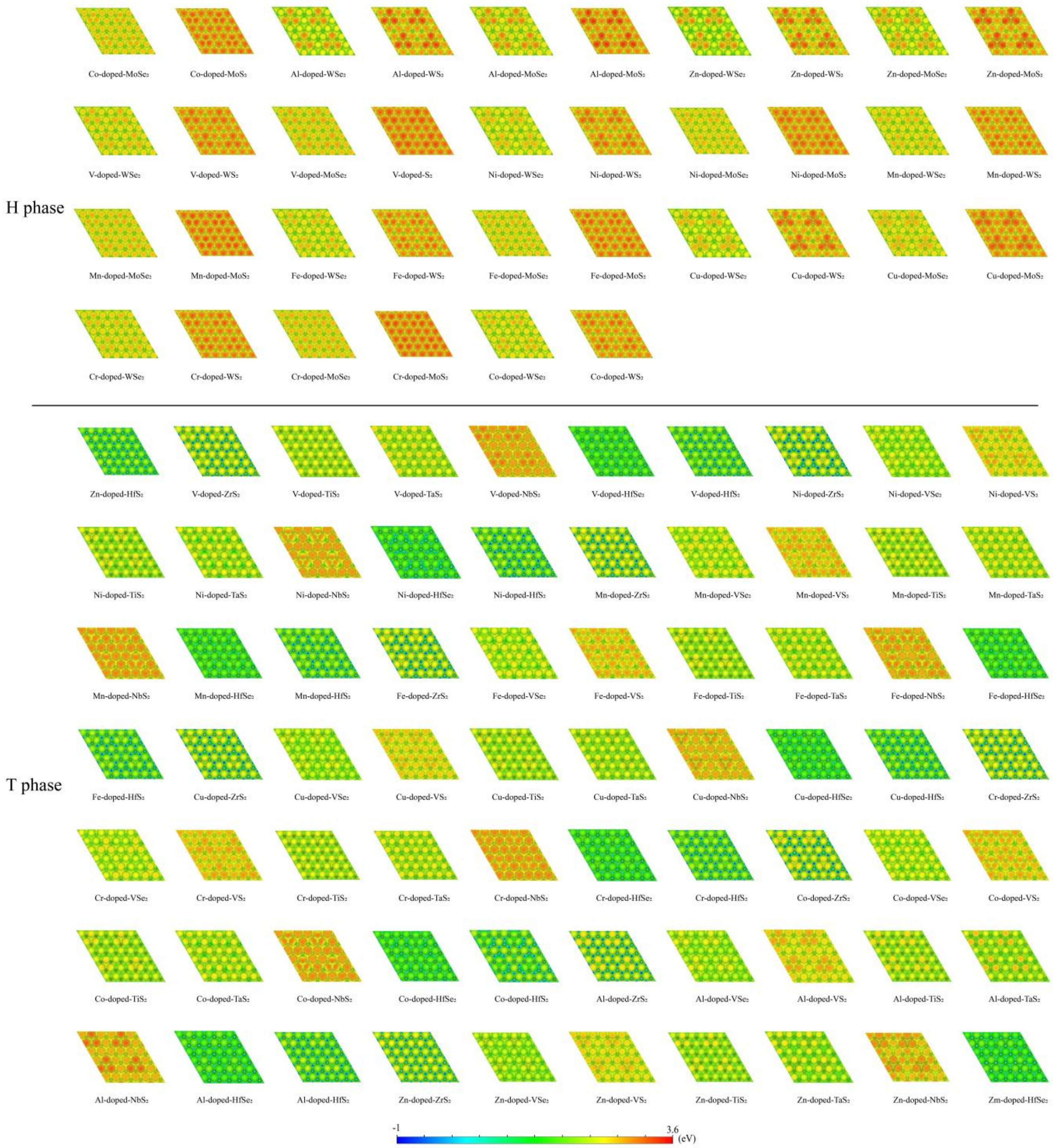

Fig. S2: The electrostatic potential distribution of 106 TMDs surfaces metal element doped

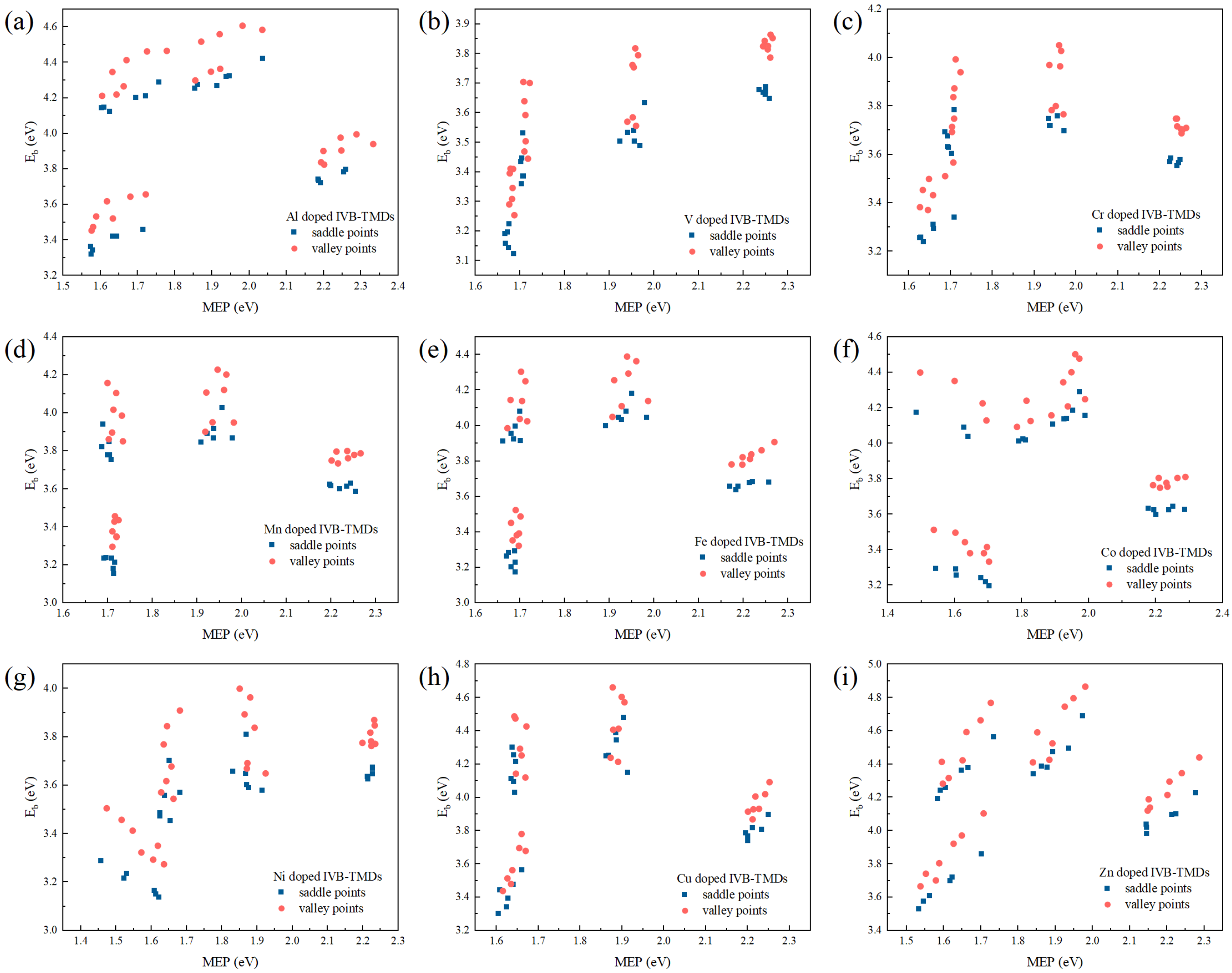

Fig. S3: Correlation between E_b of Li atoms on metal elements ((a) Al, (b) V, (c) Cr, (d) Mn, (e) Fe, (f) Co, (g) Ni, (h) Cu, (i) Zn) doped IVB-TMDs surfaces and MEP of saddle/valley points.

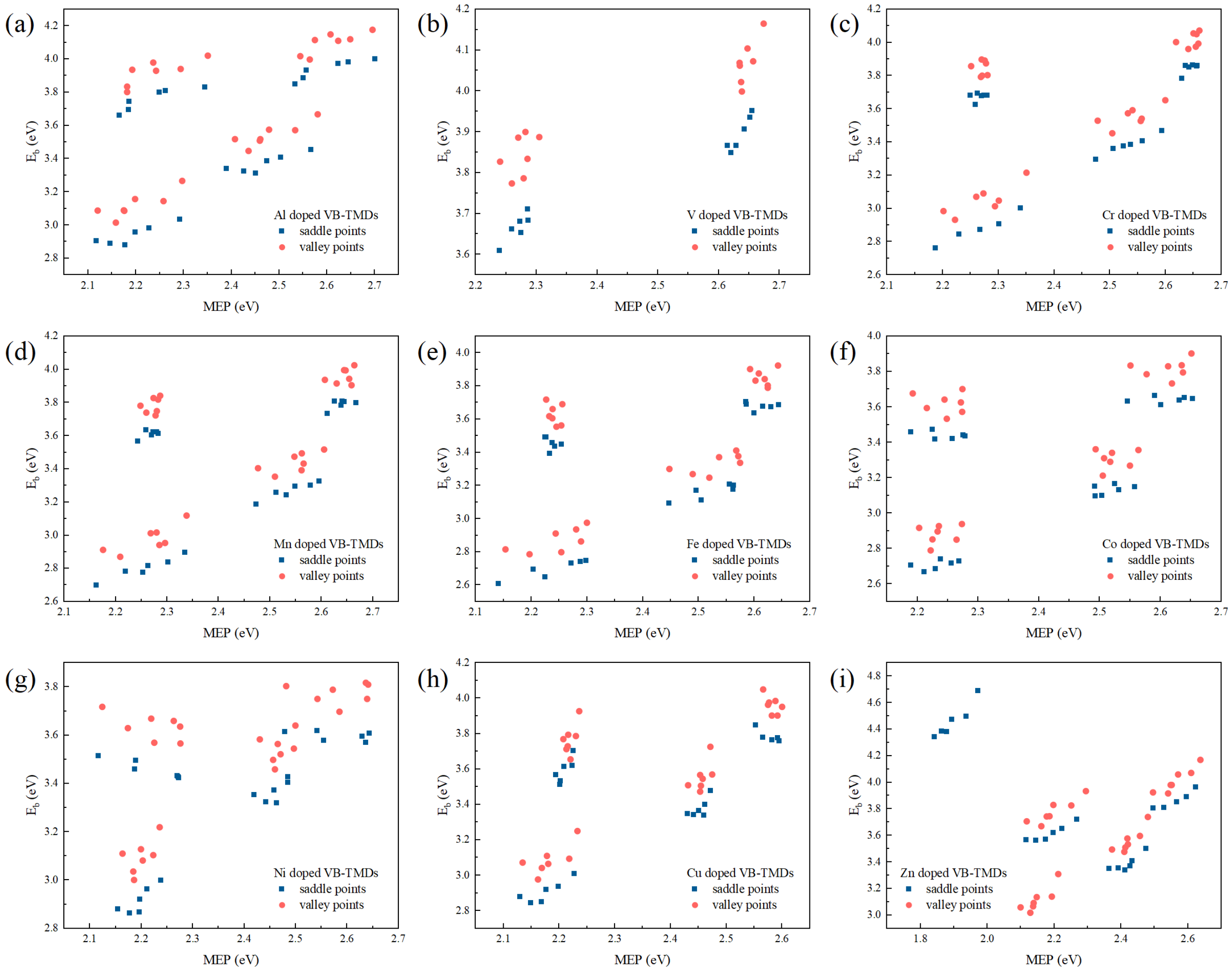

Fig. S4: Correlation between E_b of lithium atoms on metal elements ((a) Al, (b) V, (c) Cr, (d) Mn, (e) Fe, (f) Co, (g) Ni, (h) Cu, (i) Zn) doped VB-TMDs surfaces and MEP of saddle/valley points.

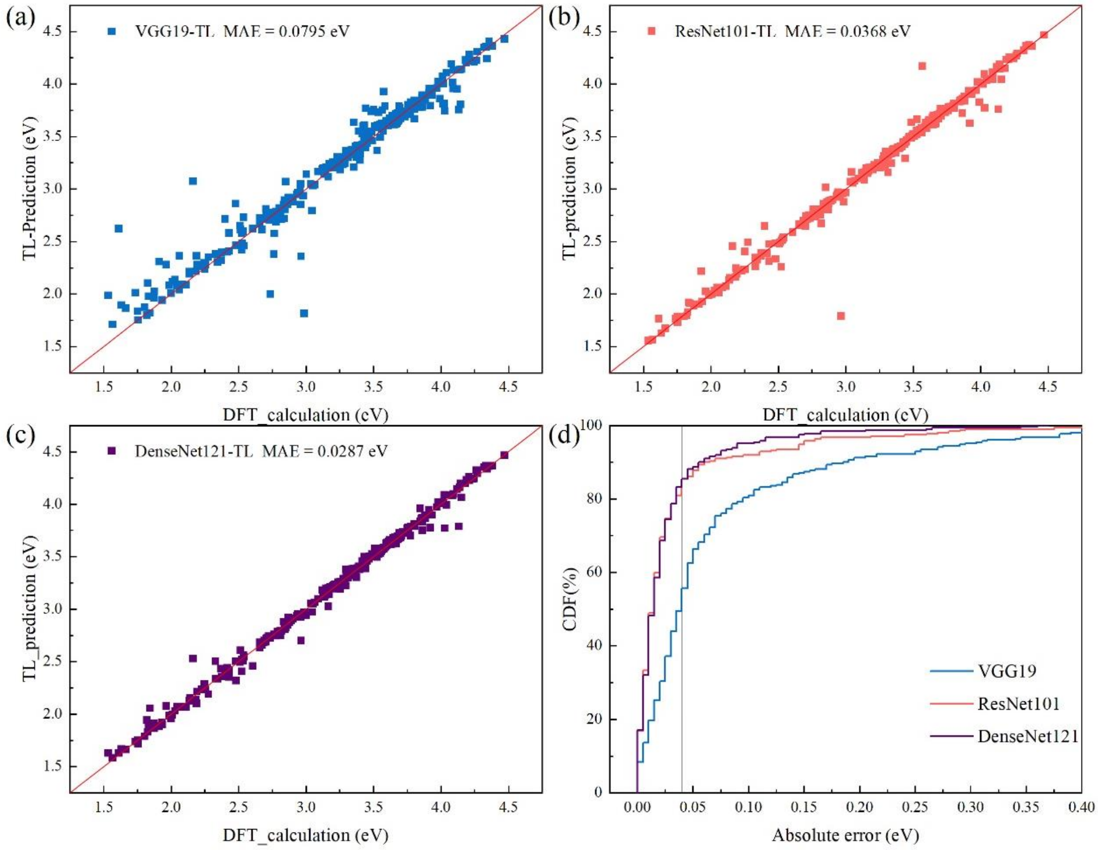

Fig. S5: The parity plot of (a) VGG19-TL, (b) ResNet101-TL and (c) DenseNet121-TL testing set, and (b) the cumulative distribution function of VGG19-TL, ResNet101-TL and DenseNet121-T

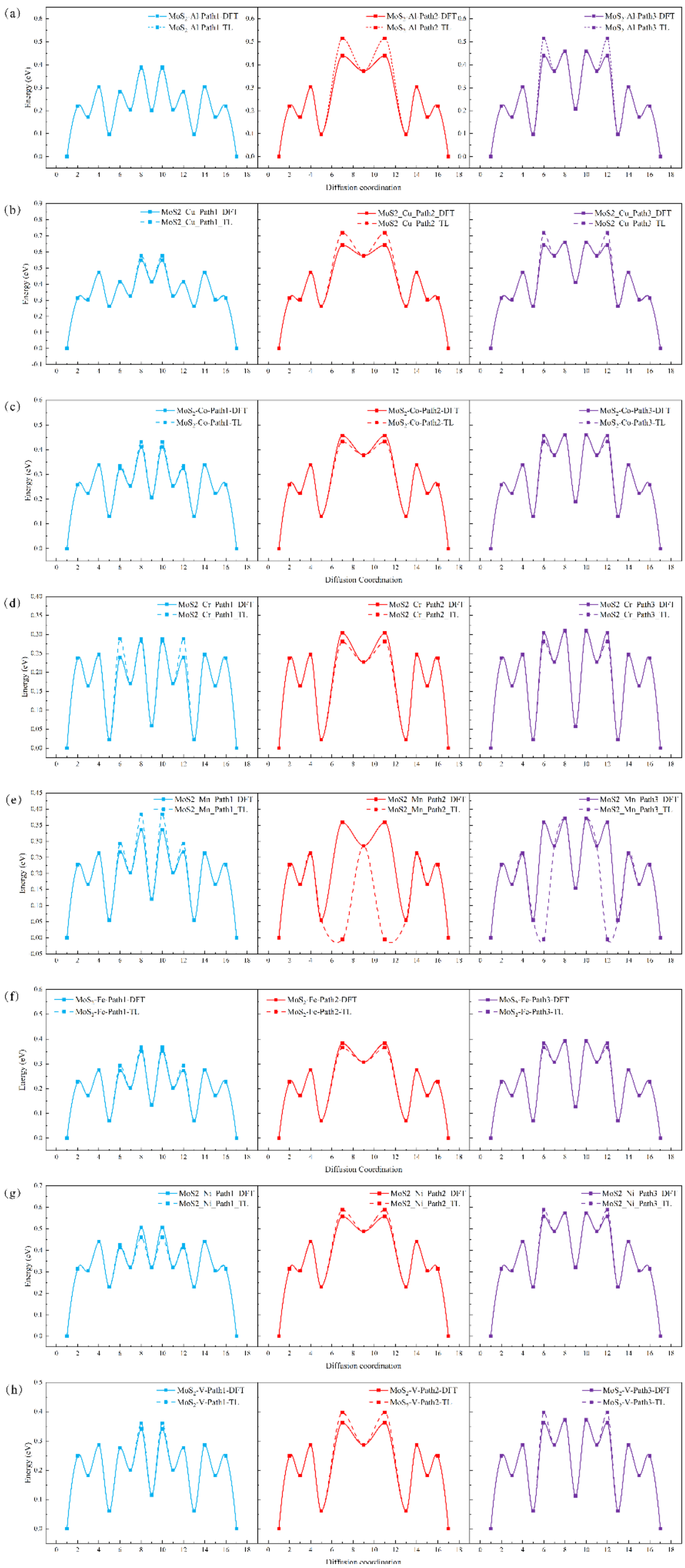

Fig. S6: The perdiction performance of lithium diffusion minimum energy profile for (a)Al, (b)Cu, (c)Co, (d)Cr, (e)Mn, (f)Fe, (g)Ni and (h)V doped MoS_2

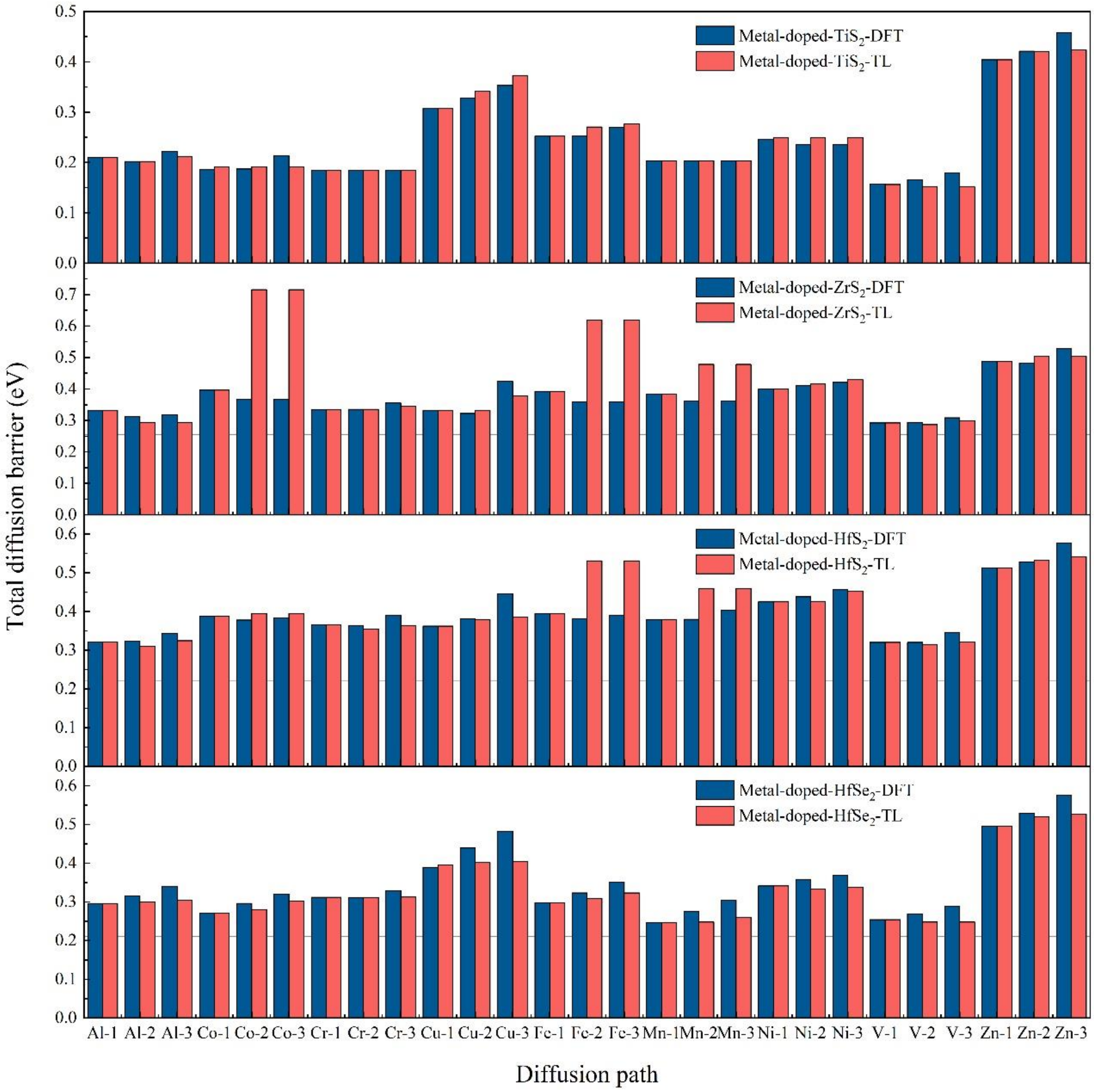

Fig. S7: The DFT calculated and TL predicted values of total diffusion barrier for metal-doped-IVB-TMDs; The reference line is the diffusion barrier of the stoichiometric surface

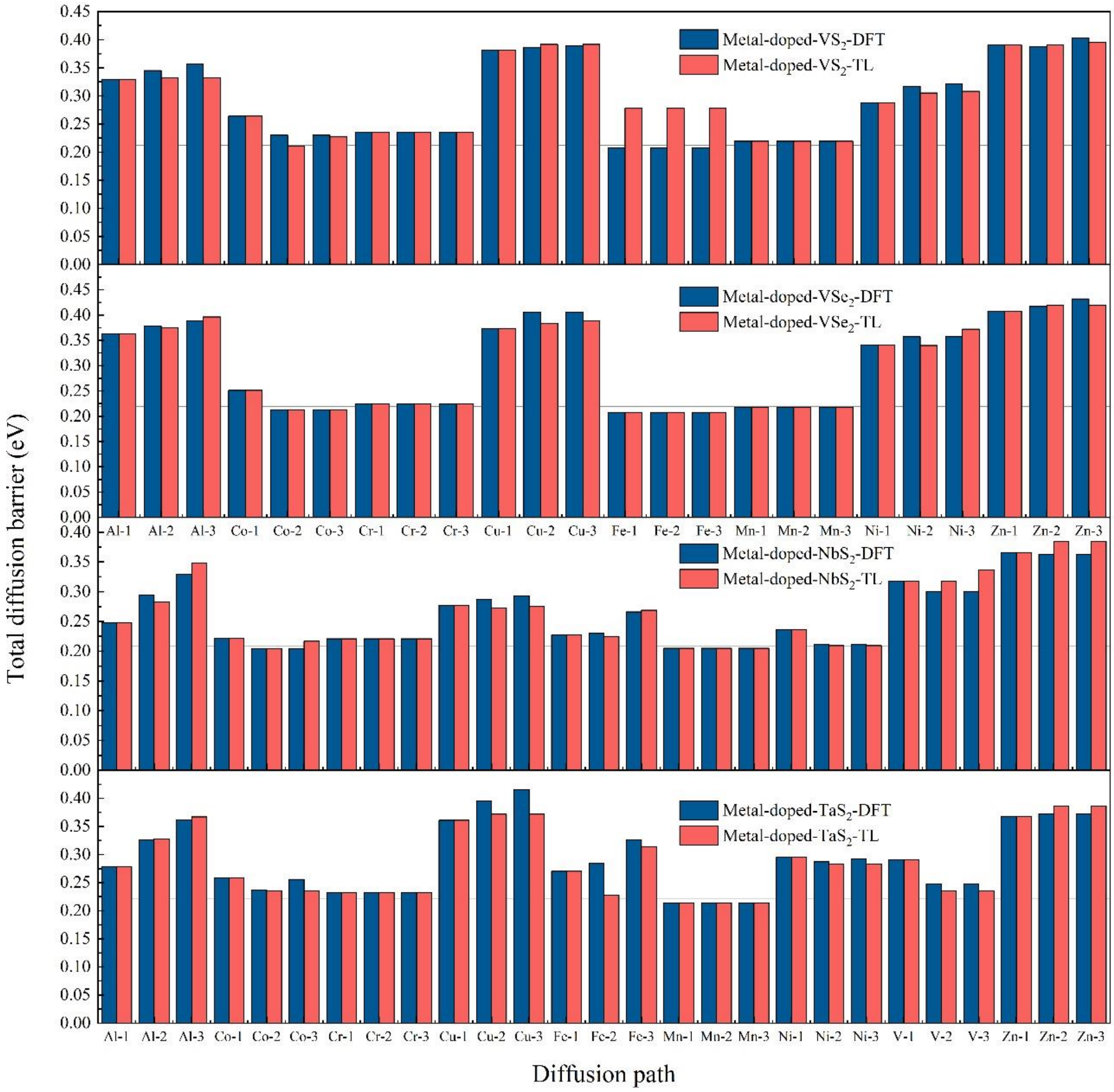

Fig. S8: The DFT calculated and TL predicted values of total diffusion barrier for metal-doped-VB-TMDs; The reference line is the diffusion barrier of the stoichiometric surface.

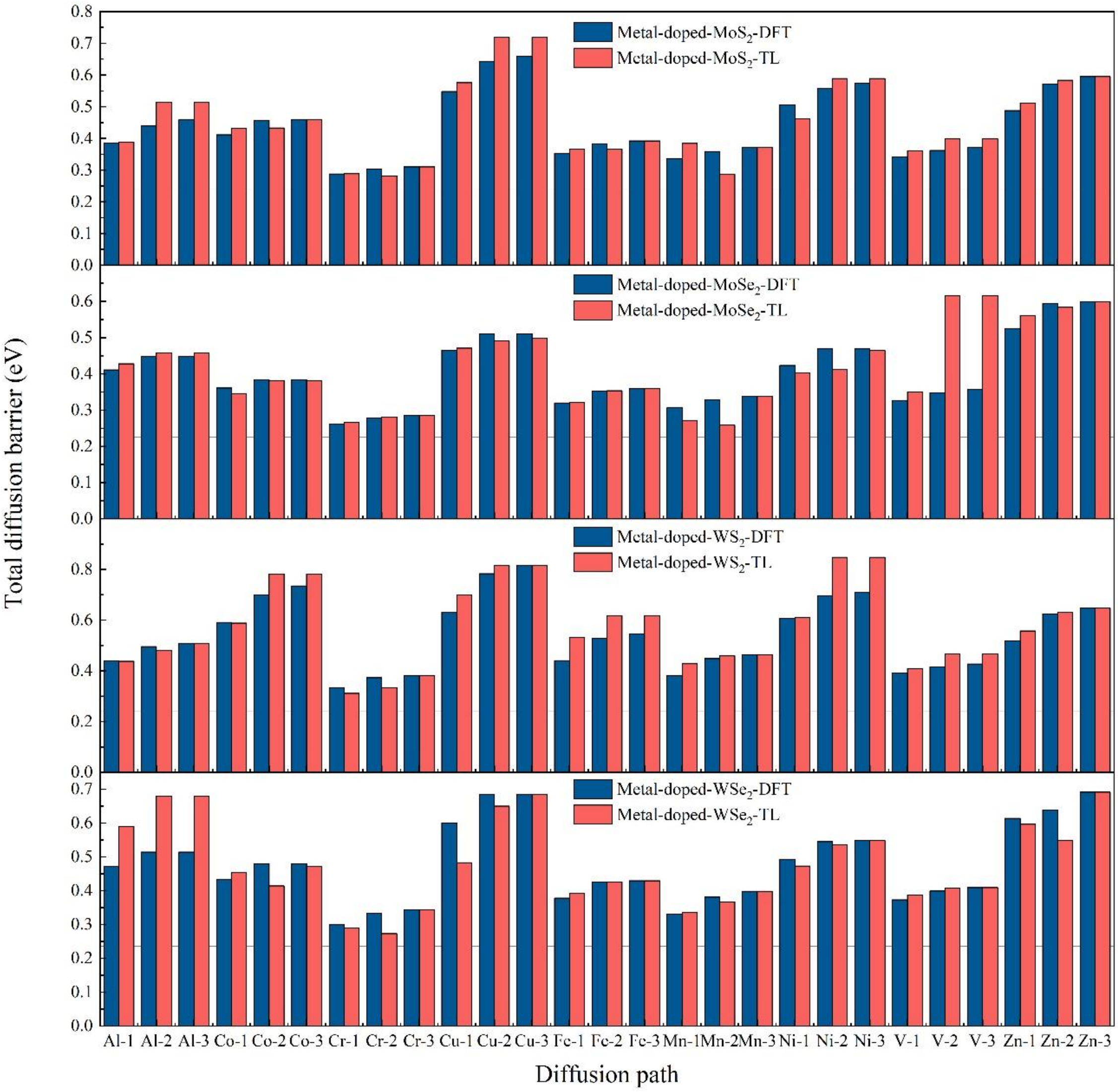

Fig. S9: The DFT calculated and TL predicted values of total diffusion barrier for metal-doped-VIB-TMDs; The reference line is the diffusion barrier of the stoichiometric surface.

Diffusion-path	E_{work} (eV)	E_{rf} (eV)V
MoS_2	0.24	0.21[1]
$MoSe_2$	0.23	0.24[2]
WS_2	0.24	0.24[2]
WSe_2	0.24	0.275[2]
VS_2	0.21	0.22[3]
VSe_2	0.22	0.33[4]
NbS_2	0.21	0.24[5]
TaS_2	0.22	0.21[6]
TiS_2	0.18	0.19[7]
ZrS_2	0.26	0.24[8]
HfS_2	0.22	
$HfSe_2$	0.21	

Table S1: Li diffusion barrier of stoichiometric TMDs surface

Github link for Python scripts of Data post-processing

https://github.com/cjone/Data-post-processing-scripts.git

References

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