Supporting Information

Novel $WS_2/NbSe_2$ vdW heterostructure as a ultrafast charging and discharging anode material for Lithium-ion batteries

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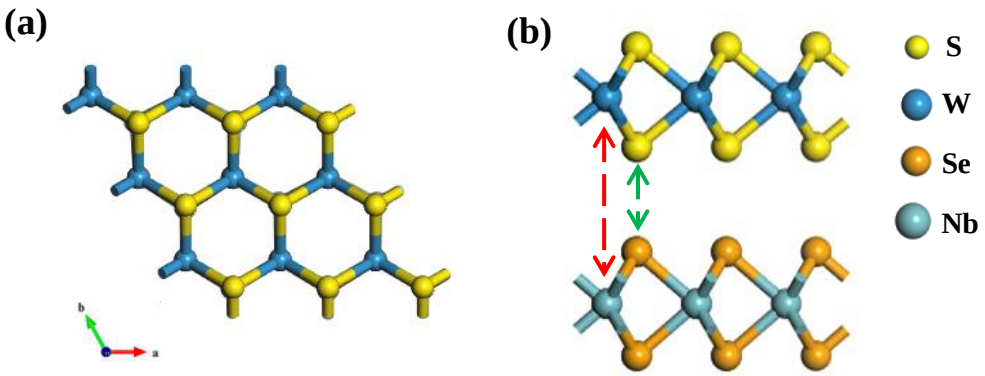

Figure S1: (a) Top and (b) side views of $WS_2/NbSe_2$ heterostructure with the AA staking. The red arrows indicate that the metal atoms in the upper layer are directly opposite the metal atoms in the lower layer, while the green ones indicate that the chalcogenide atoms in the upper layer are directly opposite the chalcogenide atoms in the lower layer.

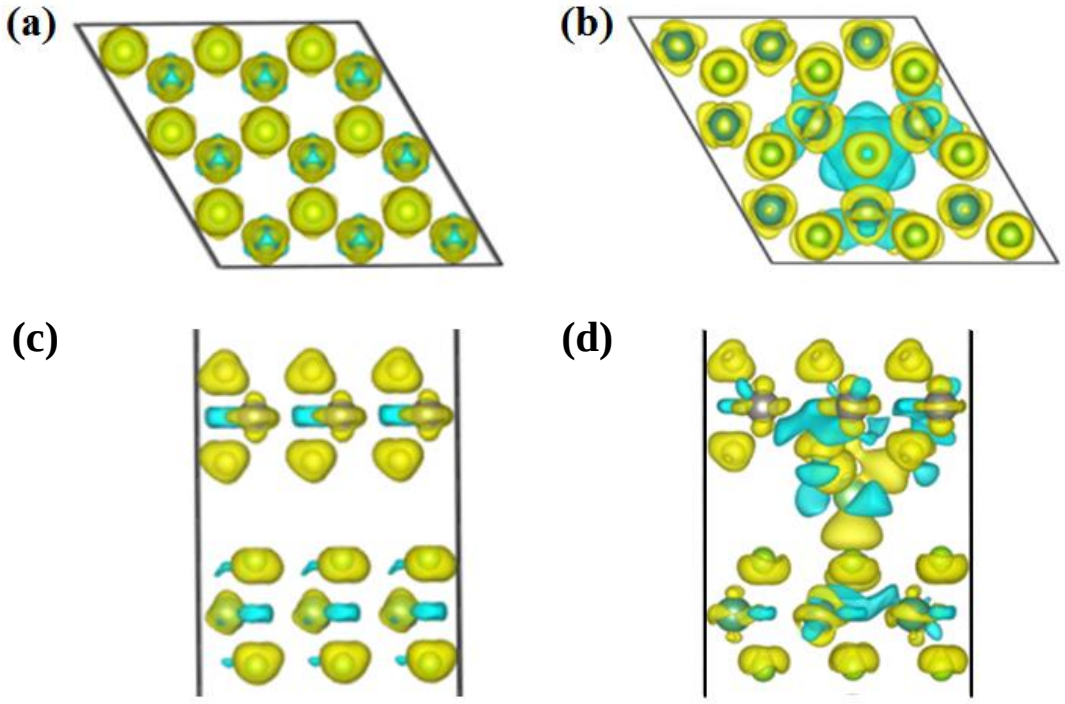

Figure S2: (a) Top and (c) side views of the charge density difference of $WS_2/NbSe_2$ heterostructure; (b) top and (d) side views of the charge density difference of one Li insert into interlayer of $WS_2/NbSe_2$ heterostructure. The loss of electrons is indicated in blue and gain of electrons is indicated in yellow.

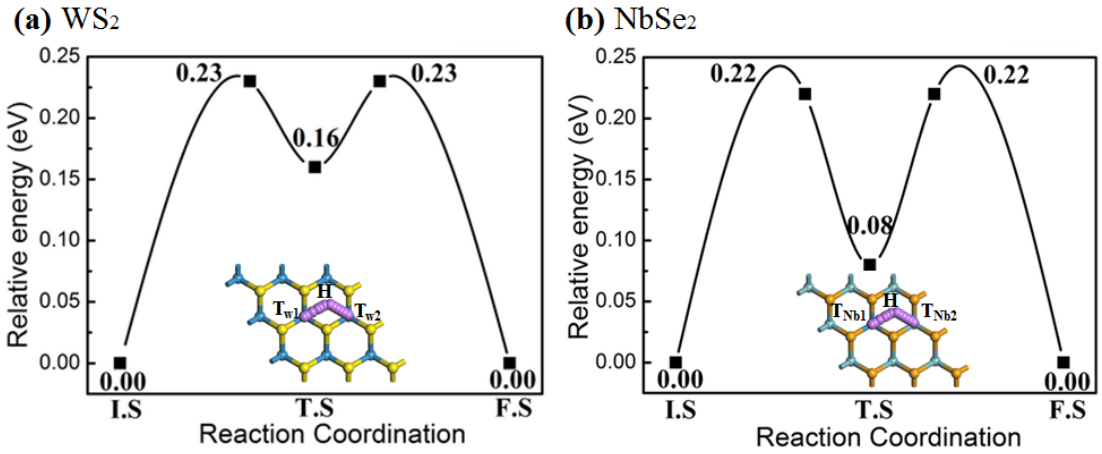

Figure S3: Considered the diffusion barrier and the shortest diffusion path (T_{W1}/T_{Nb1}-H_{WS2}/H_{NbSe2}-T_{W2}/T_{Nb2}) profiles for one Li atom adsorbed on the (a) WS_2 monolayer and (b) $NbSe_2$ monolayer.

Table S1: Calculated lattice parameters of WS_2, $NbSe_2$ monolayers and $WS_2/NbSe_2$ heterostructure, previous theoretical values values are also shown for comparison.

System	Lattice constant (Å) Calculate	Lattice constant (Å) Theory	References
WS_2	3.185	3.154	[1]
$NbSe_2$	3.337	3.481	[2]
$WS_2/NbSe_2$	3.352	-	This work

Table S2: Calculated strain energy of WS_2, $NbSe_2$ monolayers and adhesive energy of $WS_2/NbSe_2$ heterostructure.

Strain energy (eV/unit-cell)		Adhesive energy (eV/unit-cell)
WS_2	$NbSe_2$	$WS_2/NbSe_2$
0.250	0.128	0.397

Table S3: The calculated interlayer distance between $WS_2/NbSe_2$ heterojunction before and after lithium atom intercalation.

Interlayer distance (Å) $WS_2/NbSe_2$	Intrinsic	3.25
	$H_{WS2/NbSe2}$	3.27
	$T_{S/Nb}$	3.43

Table S4: The value of surface adsorption energy γ and binding energy E_b as the Li concentration $\Delta\mu$ for $WS_2/NbSe_2$ heterostructure.

$\Delta\mu$	γ (eV)	E_b (eV)
0.11	0.441	-3.19
0.33	0.372	-4.37
0.66	0.323	-4.45
1.00	0.268	-4.87

Table S5: Considered the the two diffusion paths and the corresponding diffusion barrier for one Li atom adsorbed on the WS_2, $NbSe_2$ monolayers, and insert into interlayer of $WS_2/NbSe_2$ heterostructure.

System	Path	Energy barrier (eV)	Diffusion length (Å)
$WS_2/Li_{0.11}$	T_{W1}-H_{WS2}-T_{W2}	0.23	3.48
	T_{W1}-T_{W2}	0.22	3.19
$NbSe_2/Li_{0.11}$	T_{Nb1}-H_{NbSe2}-T_{Nb2}	0.22	4.24
	T_{Nb1}-T_{Nb2}	0.20	3.51
$WS_2/Li_{0.11}/NbSe_2$	H_1-$T_{S/Nb}$-H_2	0.19	3.84
	H_1-H_2	0.18	3.40

1 A. Kumar and P. K. Ahluwalia, *Eur. Phys. J. B.*, 2012, **85**, 186.

2 X. Lv, W. Wei, Q. Sun, B. Huang and Y. Dai, *J. Phys. D.*, 2017, **50**, 23.