

Supporting Information

CrXY(X/Y = S, Se, Te) Monolayers as Efficient Anode Material for Li and Na-
Ion Batteries: A First-Principles Study

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Table S1 : Total energy of janus monolayer with and without DFT-D3 (dispersion)

Janus monolayer	Total energy without DFT – D3 method (eV)	Total energy with DFT –D3 Method (eV)
CrSSe	-24317.06	-24319.32
CrSTe	-22534.29	-22536.67
CeSeTe	-34526.41	-34529.01

Table S2: Adsorption energy(E_g) with and without DFT-D3 (dispersion)

Janus monolayer	E_g Li (eV) with DFT-D3	E_g Li (eV) without DFT-D3	E_g Na (eV) with DFT-D3	E_g Na (eV) without DFT-D3
CrSeTe	-2.23	-2.01	-1.67	-1.38

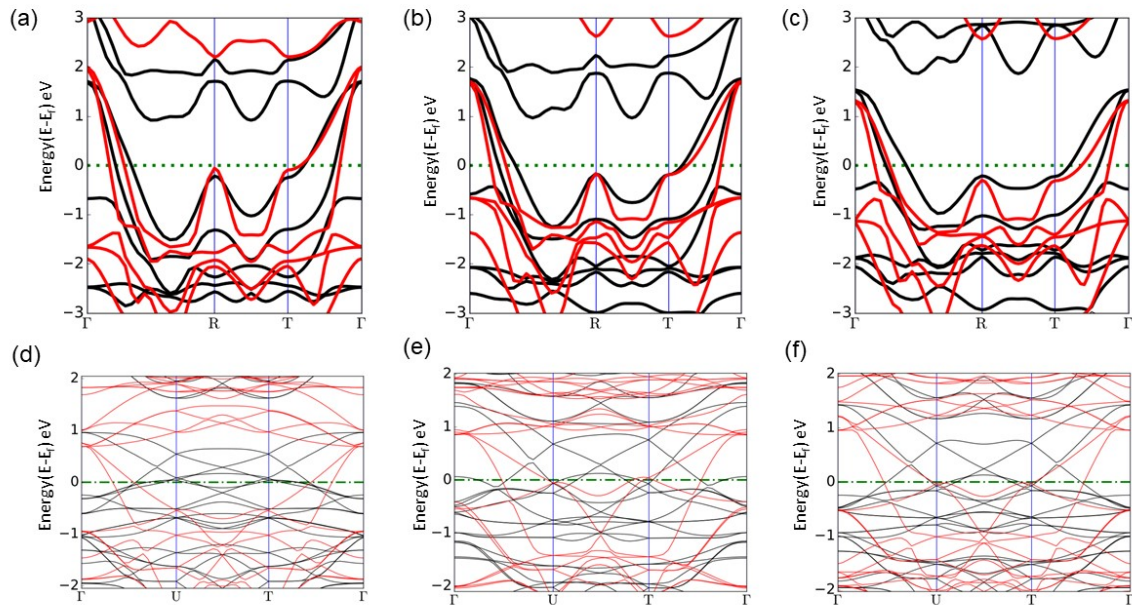


Fig S1: (a) (b), (c) Band structure of CrSSe, CrSTe and CrSeTe with PBE functional, (d), (e) and (f) band structure of CrSSe, CrSTe and CrSeTe with HSE functional

Table S3: Band gap of Janus monolayer and Adsorption energy(E_g) of Li and Na on H site with PBE and HSE functional

Janus Monolayer	HSE Bandgap E_g (eV)	PBE Bandgap(eV)	E_g (Li) by HSE (eV)	E_g (Li) by PBE (eV)	E_g (Na) by HSE (eV)	E_g (Na) by PBE(eV)
CrSSe	0	0	-1.93	-1.86	-1.09	-1.01
CrSTe	0	0	-1.72	-1.66	-1.28	-1.20
CrSeTe	0	0	-2.23	-2.15	-1.67	-1.56

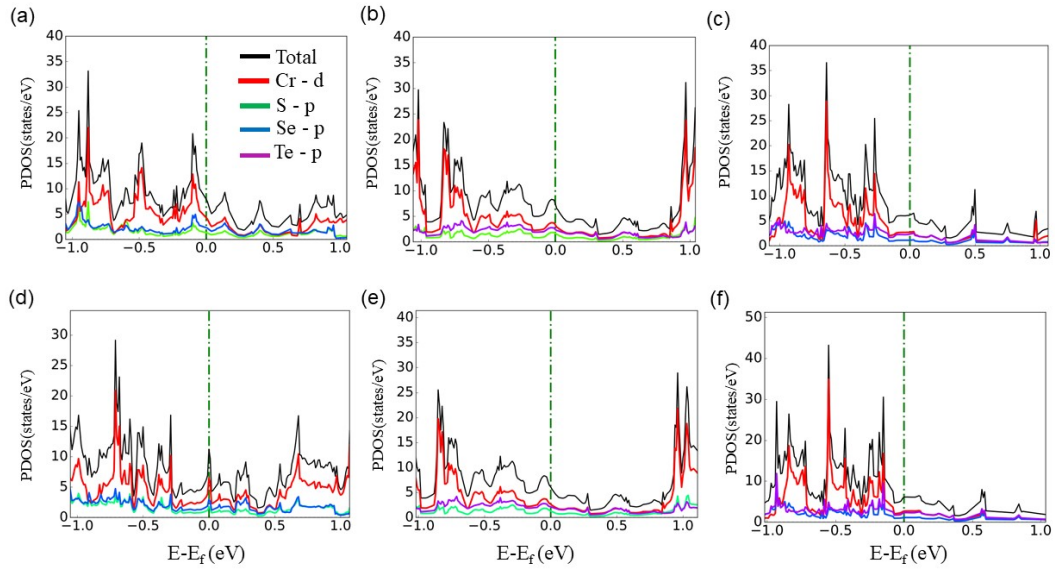


Fig S2 :(a) (b), (c) PDOS of CrSSe, CrSTe and CrSeTe with PBE with Fermi-Dirac occupation, (d), (e) and (f) PDOS of CrSSe, CrSTe and CrSeTe with Methfessel-Paxton

Table S4: Band gap and adsorption energy at different lattice constant

Janus CrSSe at lattice constant c (Å)	Bandgap (eV)	Adsorption energy of Li (eV)	Adsorption energy of Na (eV)
15	0	-1.8601	-1.01004
17	0	-1.8600	-1.01004
20	0	-1.8601	-1.01003

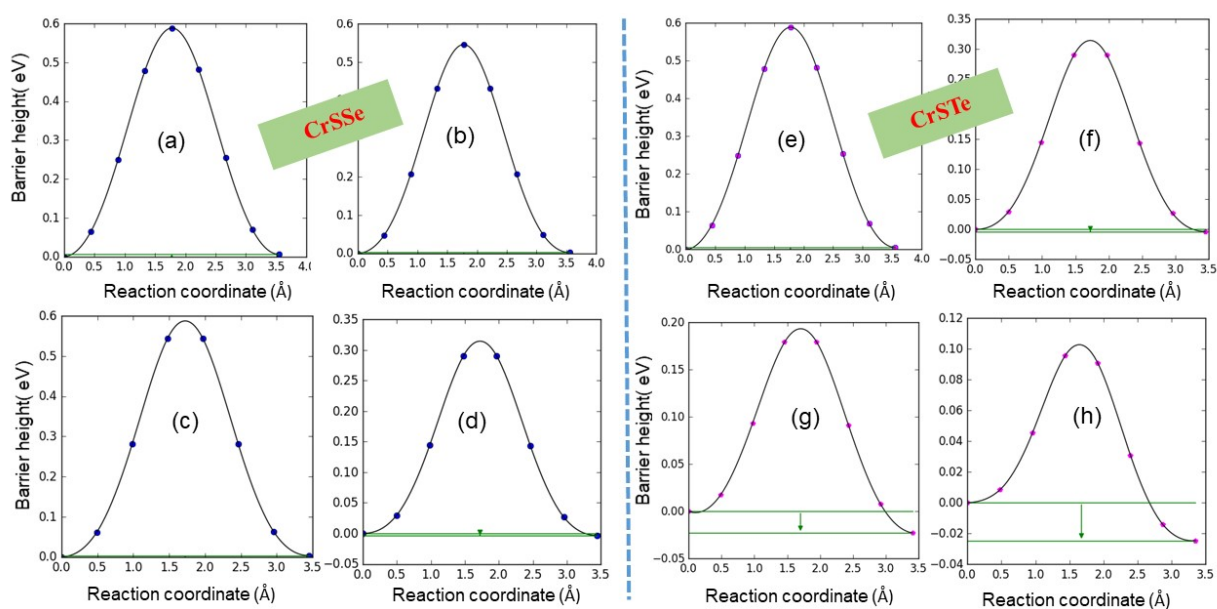


Fig S3: (a),(b) and (c), (d) Diffusion barrier of Li and Na above S layer and below Se layer for CrSSe monolayer respectively. (e),(f) and (g), (h) Diffusion barrier of Li and Na above S layer and below Te layer for CrSTe monolayer respectively

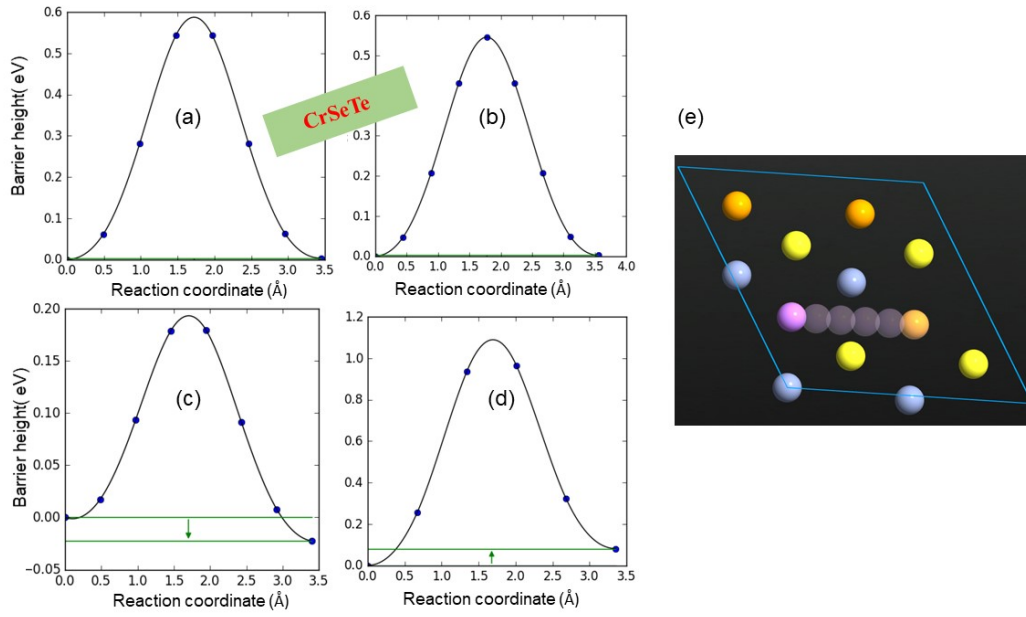


Fig S4: (a),(b) and (c), (d) Diffusion barrier of Li and Na above Se layer and below Te layer for CrSeTe monolayer respectively, (e) schematic of the diffusion path