

Supporting Information for Tunable Li-ion diffusion properties in MoSSe bilayer anode by strain gradient

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Snapshots from AIMD simulations on pristine MoSSe bilayers.

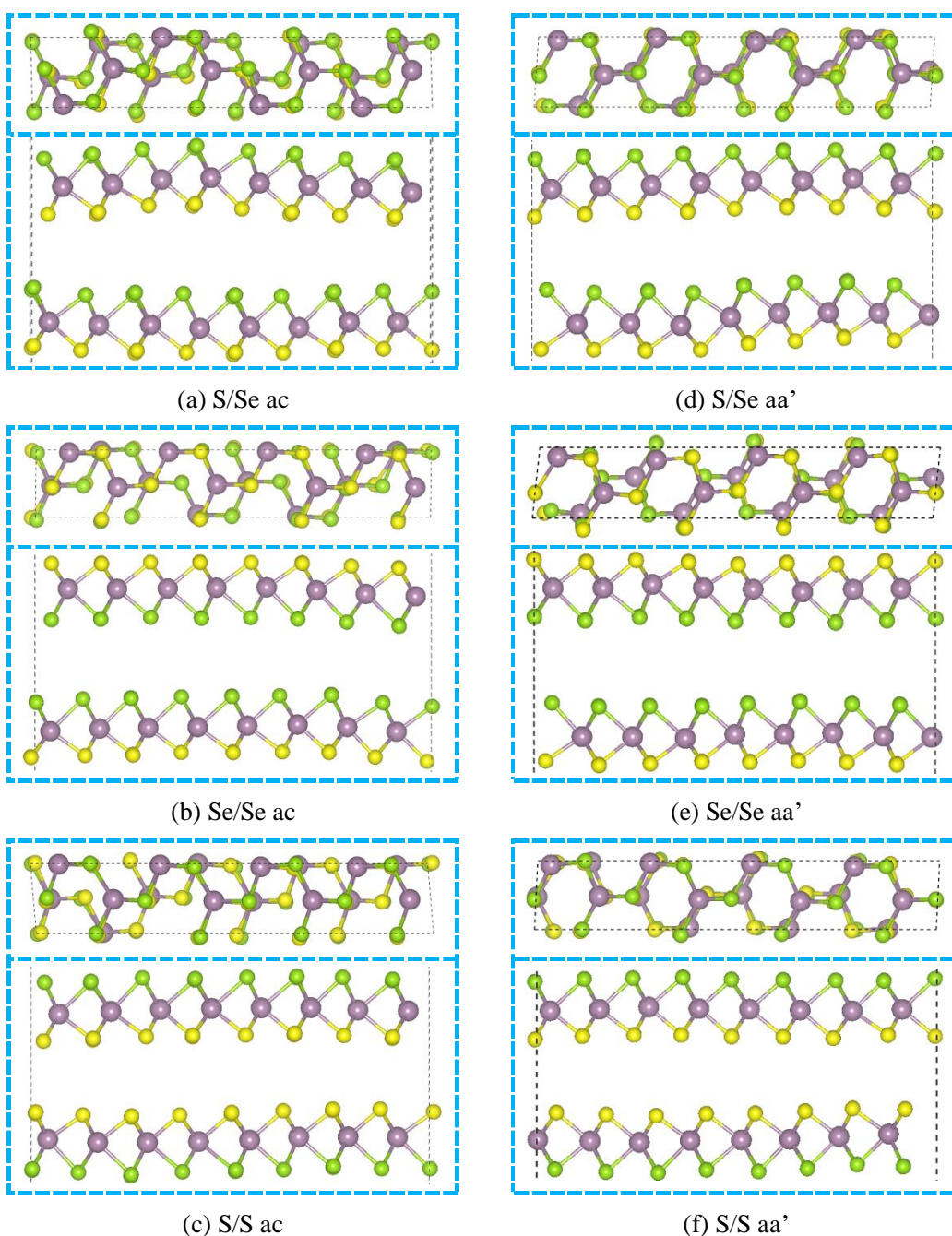


Fig. S1. The captured snapshots from AIMD simulations at 300 K and 25 ps for pristine (a) S/Se ac, (b) Se/Se ac, (c) S/S ac (d) S/Se aa', (e) Se/Se aa' and (f) S/S aa' stacking models.

Energy oscillations and associated snapshots for MoS₂Se bilayers under loads in AIMD simulations.

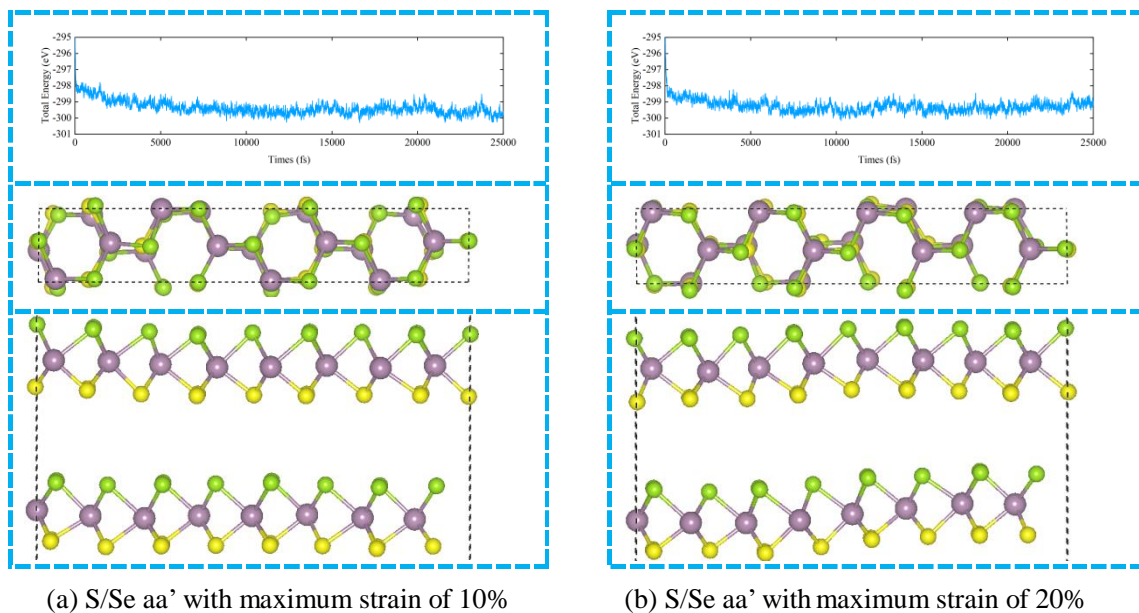


Fig. S2. The energy oscillations from AIMD simulations and associated snapshots (top and side views) at 300 K for S/Se aa' under strain gradient with maximum strains of (a) 10% and (b) 20%.

Possible adsorption sites of Li ions on MoS₂Se bilayer models.

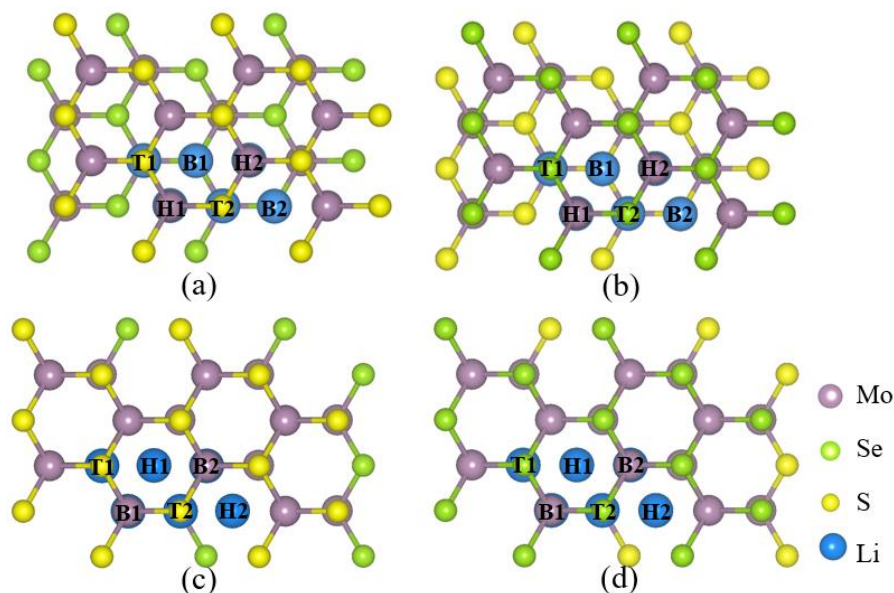


Fig. S3. Possible adsorption sites of Li ions on MoS₂Se bilayer with stacking patterns of (a) Se/Se ac, (b) S/S ac, (c) Se/Se aa' and (d) S/S aa'.

Adsorption energies of multiple Li ions on MoS₂ bilayer.

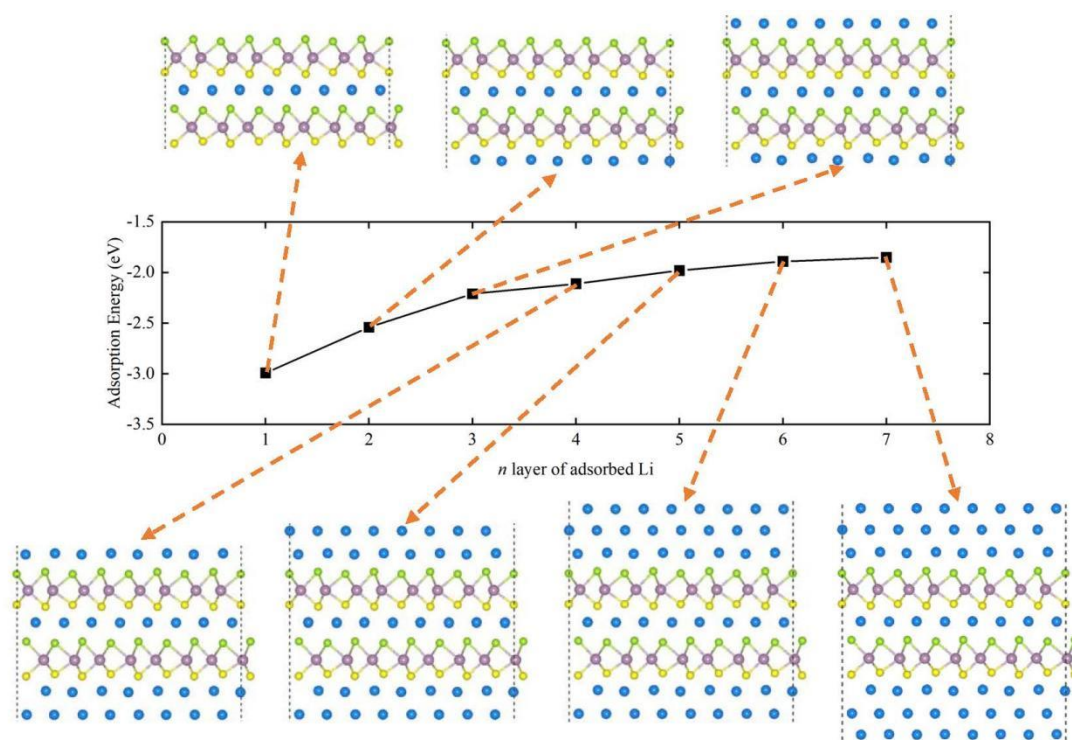
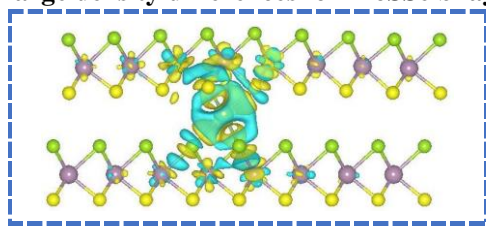
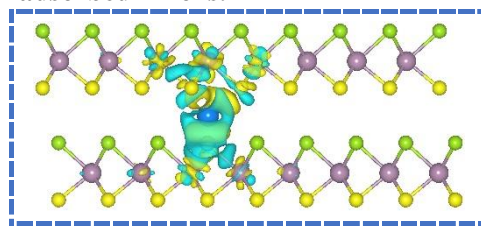


Fig. S4. Adsorption energies of Multilayer Li ions on MoS₂ bilayer.

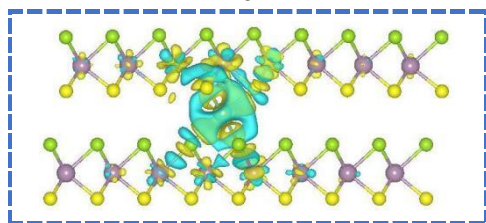
Charge density differences for MoSSe bilayer with adsorbed Li ions.



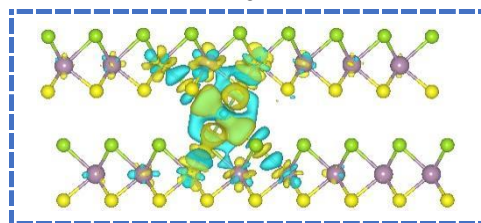
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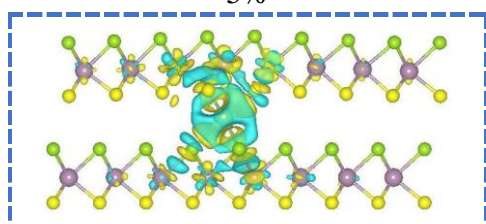
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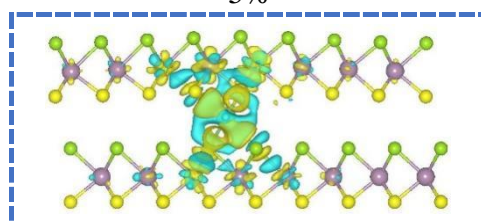
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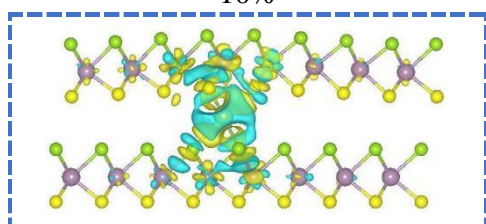
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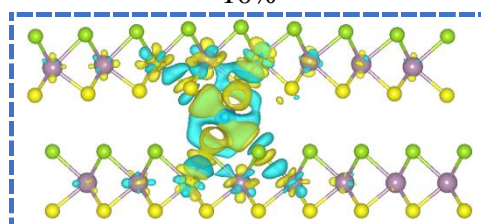
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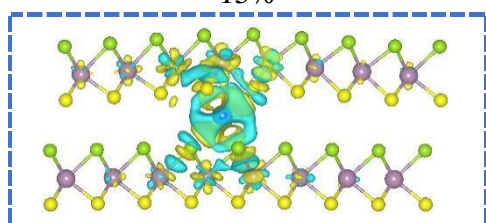
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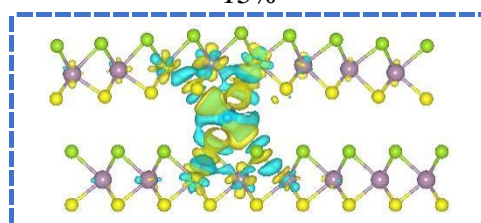
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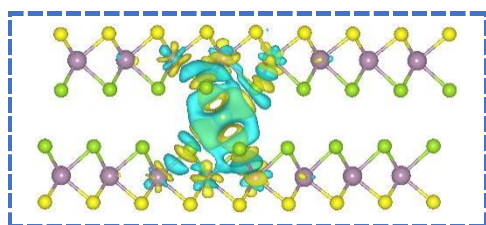
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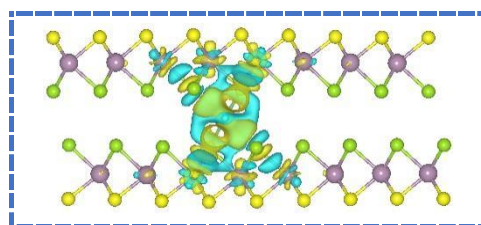
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(a) S/Se ac

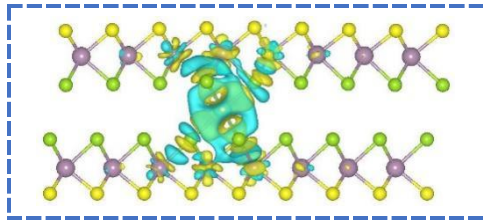
(b) S/Se aa'



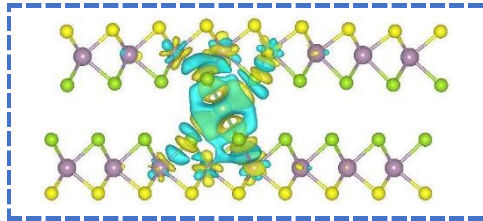
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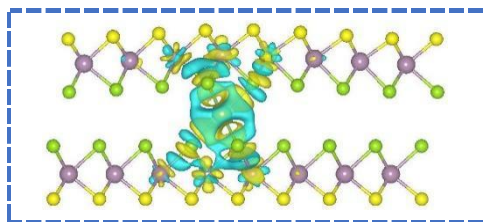
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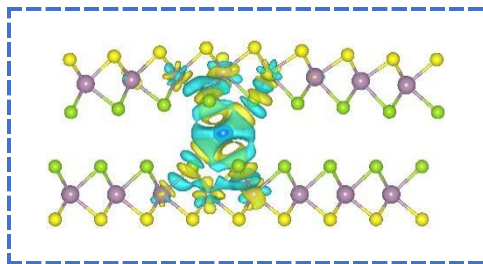
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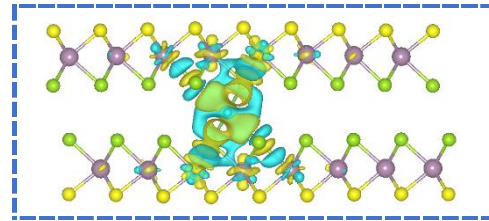


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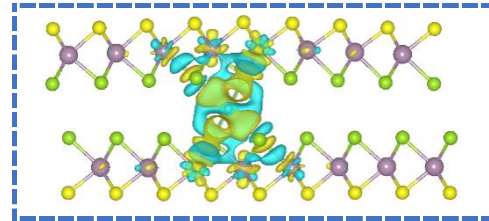


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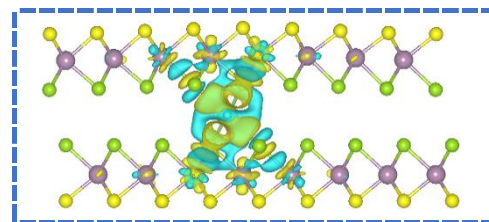
(c) Se/Se ac



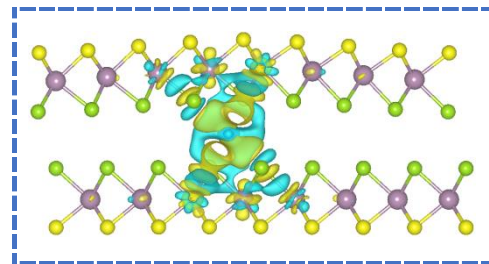
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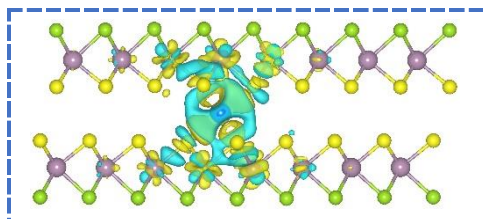


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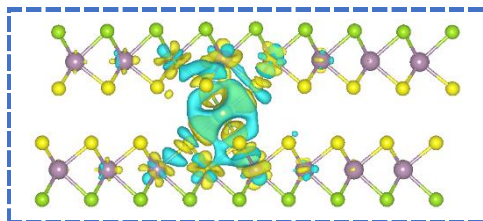


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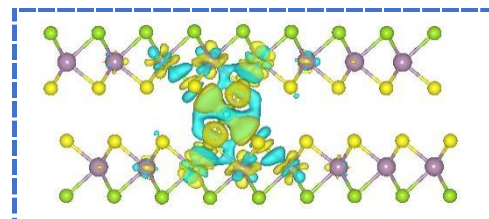
(d) Se/Se aa'



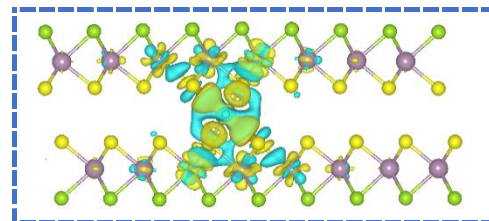
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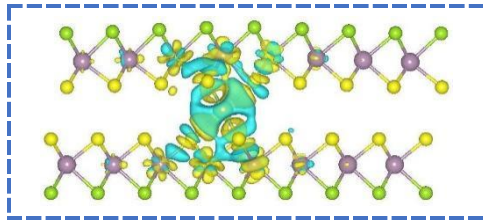
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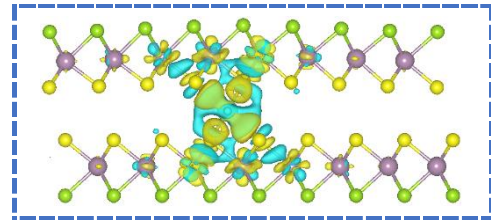
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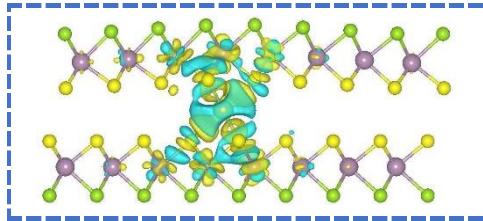
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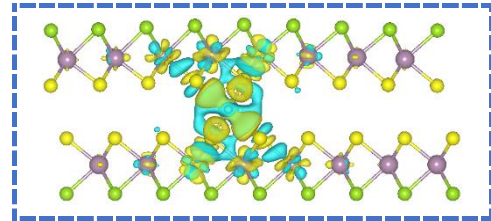
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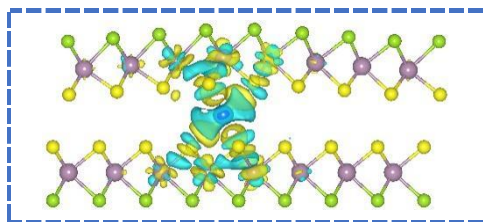
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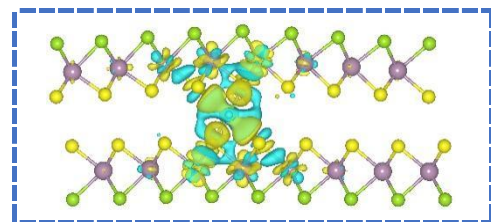
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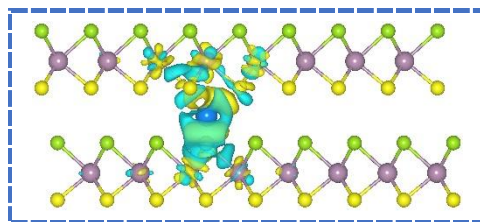
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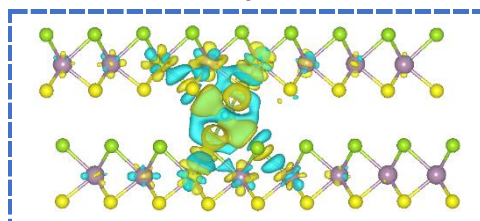
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(e) S/S ac

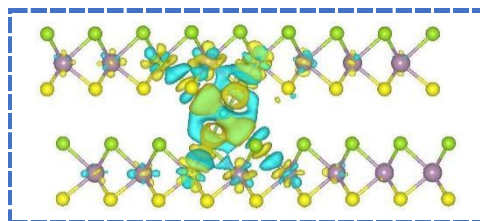
(f) S/S aa'



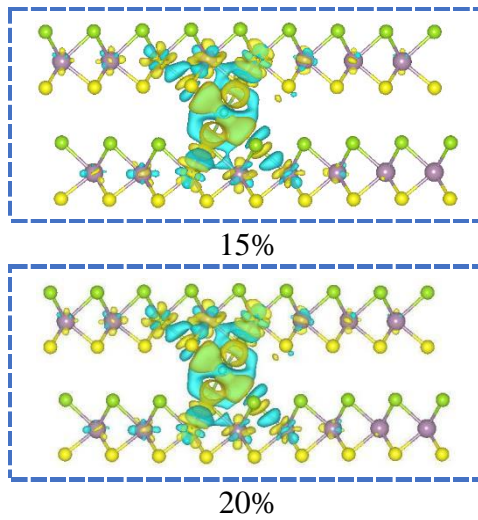
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(g) S/Se aa'(uniform strain)

Fig. S5. Charge density difference plots (side views) for the adsorption of a Li ion on MoSSe bilayer with different stacking and loads. The yellow color indicating charge accumulation and blue color representing charge depletion.