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Electronic Supplementary Information for

Lattice-Distorted Lithiation Behavior of Square Phase Janus MoSSe Monolayer for Electrode Applications

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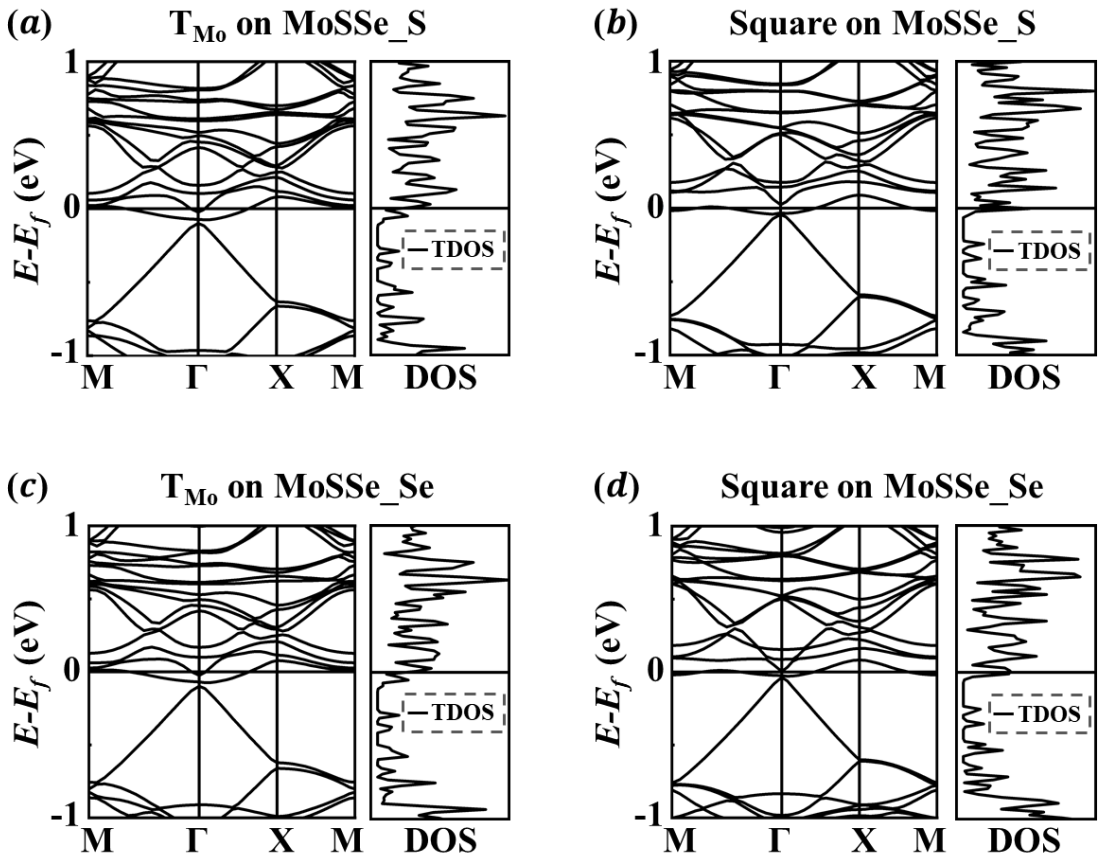

Figure S1. Electronic band structure and total density of states of system with Li adsorbed on S side at T_{Mo} site (a), square site (b), and on Se side at T_{Mo} site (c), square site (d).

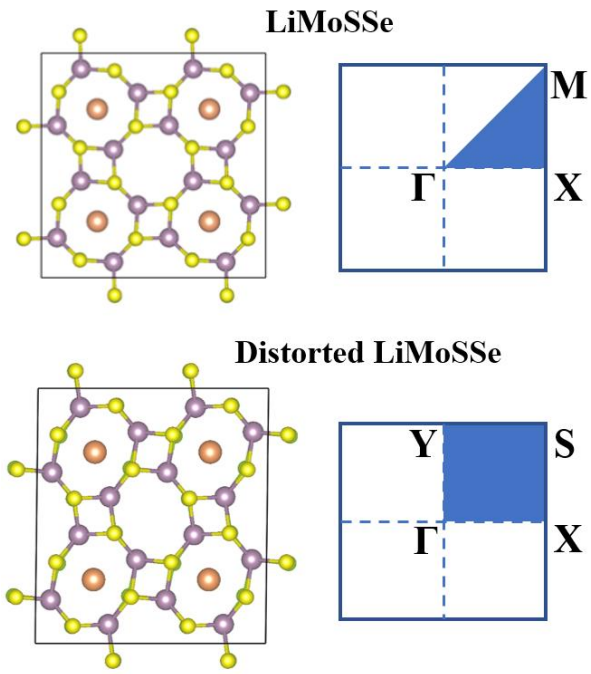

Figure S2. High symmetric points for LiMoSSe and distorted LiMoSSe in the phonon dispersion calculations.

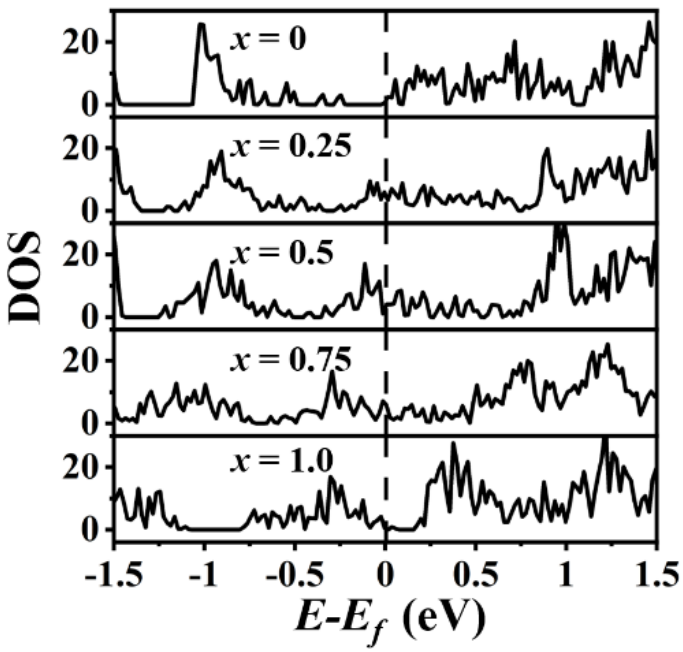

Figure S3. Total density of states of LiMoSSe. For x=0.25, 0.5 and 0.75, the distorted structures are adopted.