

# The effects of in-plane strains on the electrochemical properties of Li adatoms on the ZrS<sub>2</sub> monolayer: A first-principles study

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## 1. Supplementary-Materials

### 2. Optimized geometries of Li concentration adsorbed on a ZrS<sub>2</sub> monolayer

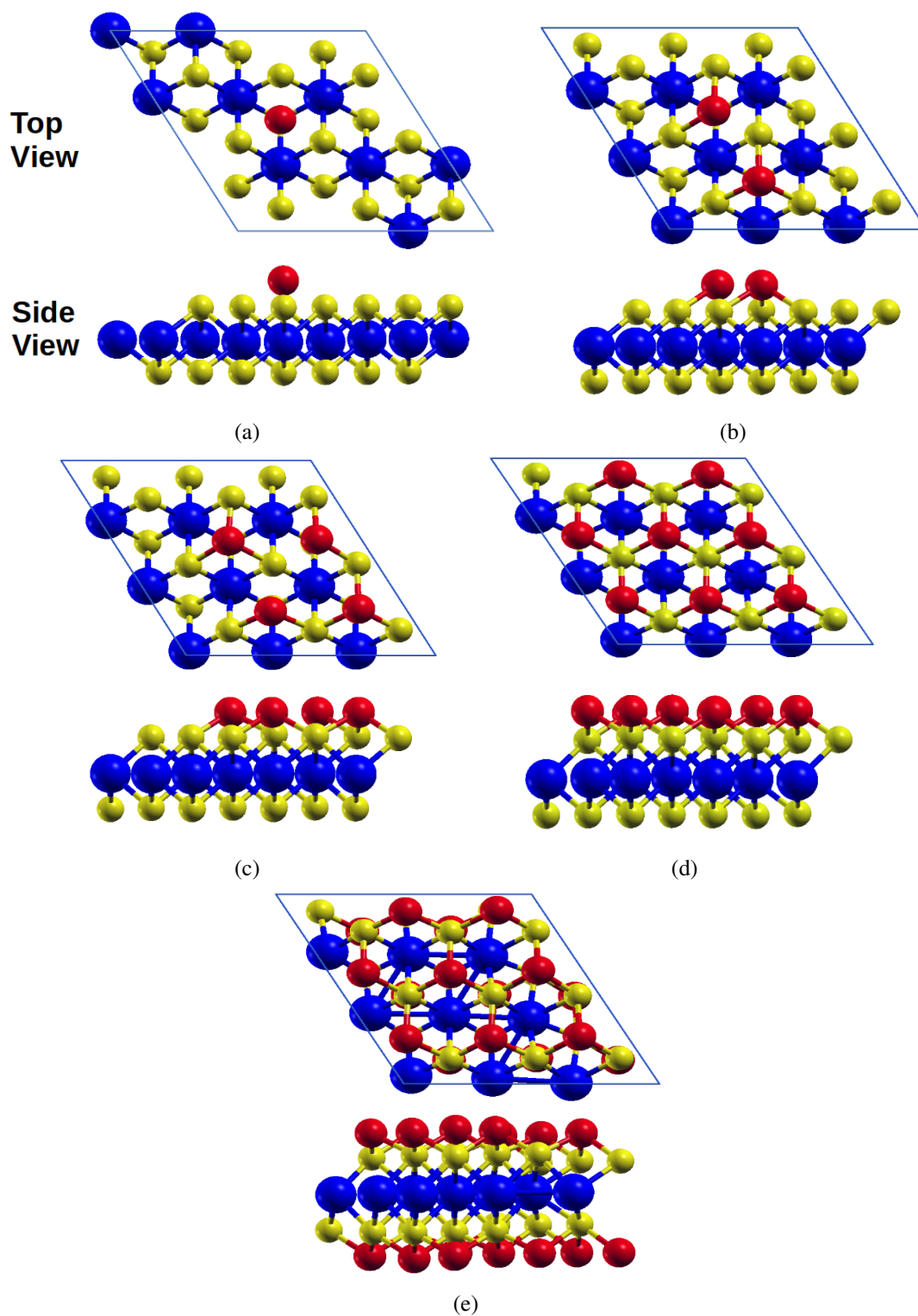


Fig. S1. The optimized configurations of lithium concentrations on ZrS<sub>2</sub> monolayer: (a) 1 Li, (b) 2 Li, (c) 4 Li, (d) 8 Li, and (e) 16 Li.

2.1. Charge density distributions of Li on a ZrS<sub>2</sub> monolayer at 0%, -5% and +5% strains.

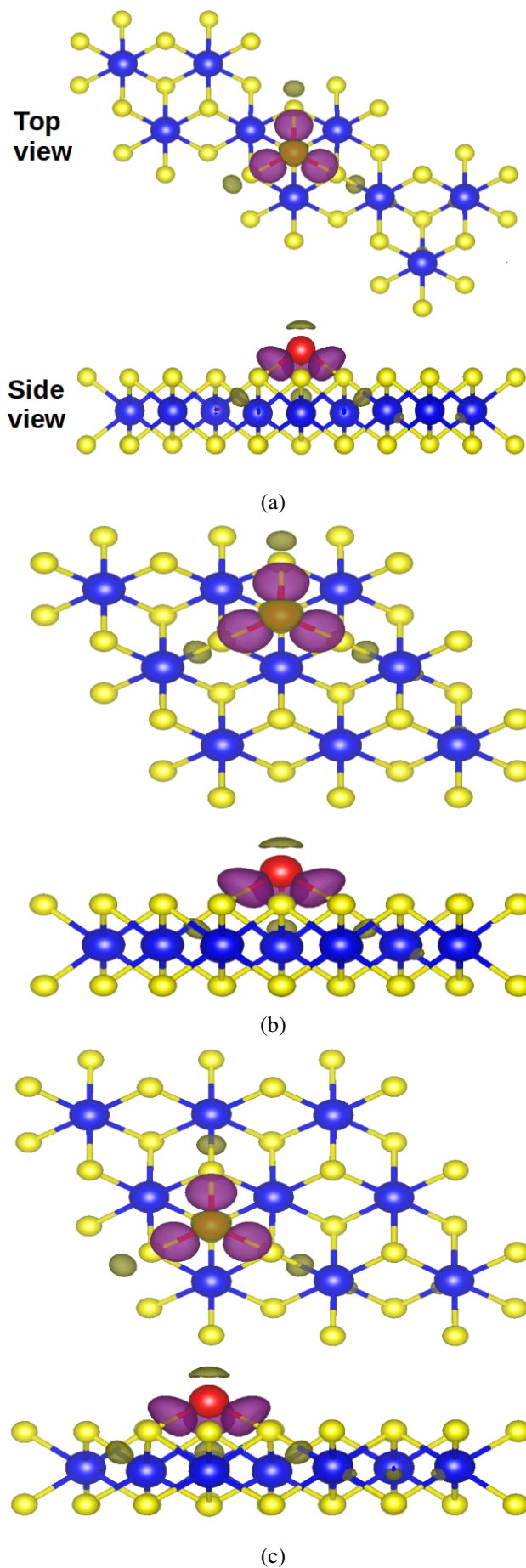


Fig. S2. The charge density distributions of Li on monolayer at different strains: (a) 0%, (b) -5%, and (c) +5%. Where pink and brown colors denote charge accumulation and depletion, respectively.