# Supporting Information for

# Are Sodiation/De-Sodiation Reactions Reversible in Two-Dimensional Metallic $NbSe_2$?

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**This PDF file includes:**

Figs. S1 to S9

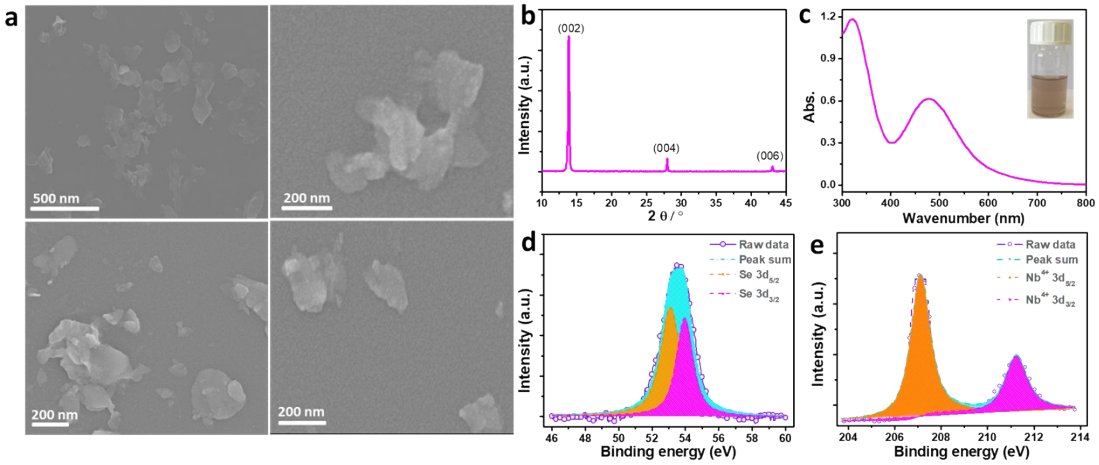


**Fig. S1** (a) SEM images of exfoliated $NbSe_2$ samples with different magnifications. (b) XRD pattern of exfoliated $NbSe_2$ samples. (c) UV absorbance spectrum of exfoliated $NbSe_2$ samples. The insert is a photograph of typically $NbSe_2$ flake dispersion. XPS spectra of (d) Se 3d and (e) Nb 3d peaks from $NbSe_2$ flakes. The Se species can be fitted with Se $3d_{5/2}$ (53.2 eV) and Se $3d3_{/2}$ (54.1 eV) peaks in agreement with the $Se^{2+}$ state. The two peaks at 203.0 and 206.5 eV correspond to the $Nb^{4+}$ state.

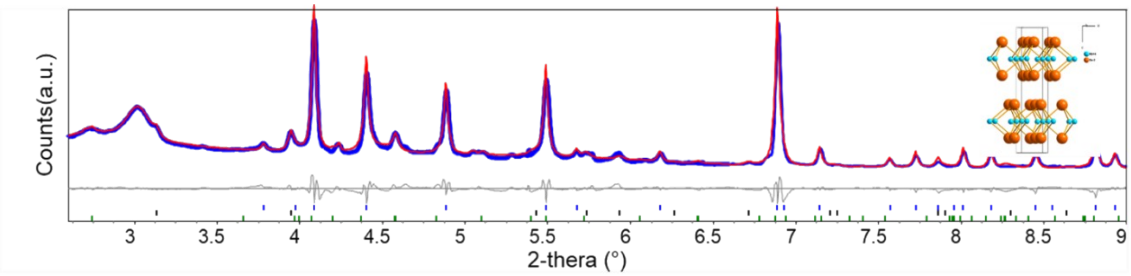


**Fig. S2** Synchrotron XRD patterns of $NbSe_2$ flakes and Rietveld analysis.

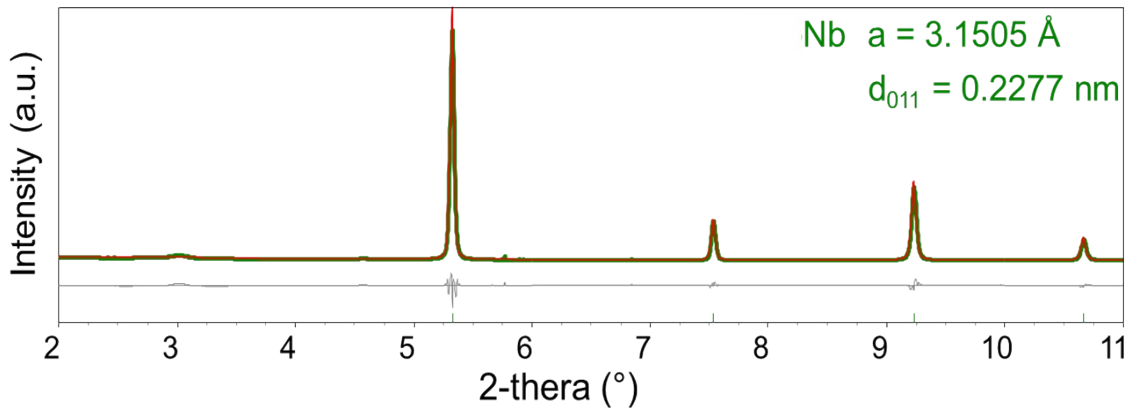


**Fig. S3** Synchrotron XRD patterns of Nb metal reference and Rietveld analysis.

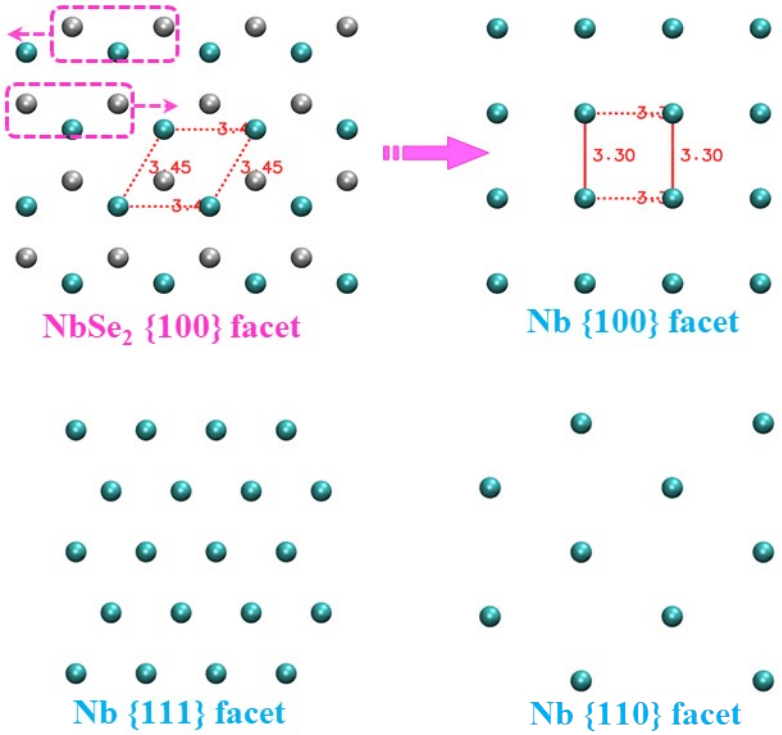


**Fig. S4** Schematic illustration of the topotactic conversion reaction and lattice models of Nb atoms in the crystal structures of $NbSe_2$ (4 × 4 supercells with 48 atoms) and *bcc* Nb (4 × 4 supercells with16 atoms in the surface layer). The grey and blue spheres represent Se and Nb atoms, respectively.

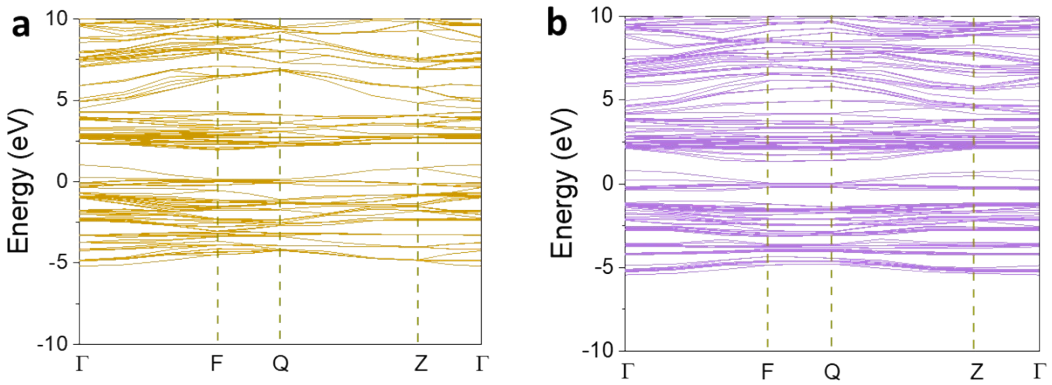


**Fig. S5** Band structures of (a) $NbSe_2$ and (b) $Na_xNbSe_2$.

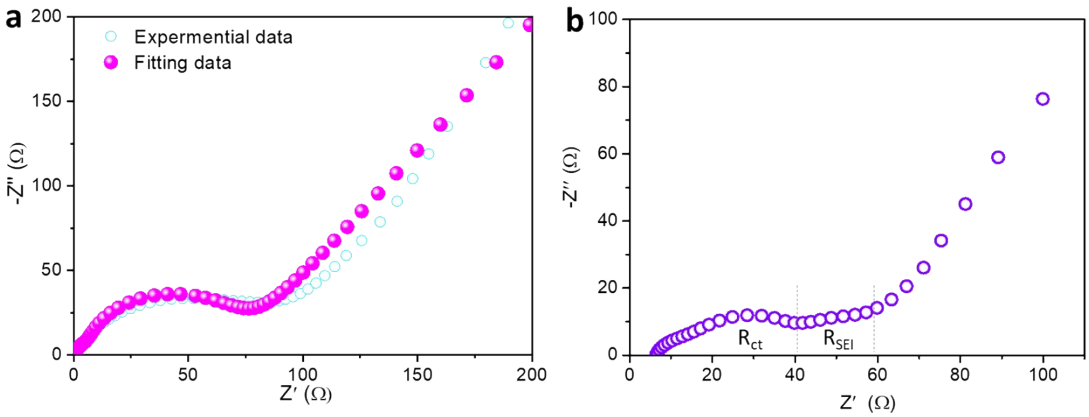


**Fig. S6** Electrochemical impedance spectroscopy (EIS) of (a) pristine $NbSe_2$ electrodes and (b) $NbSe_2$ electrode after 240 cycles.

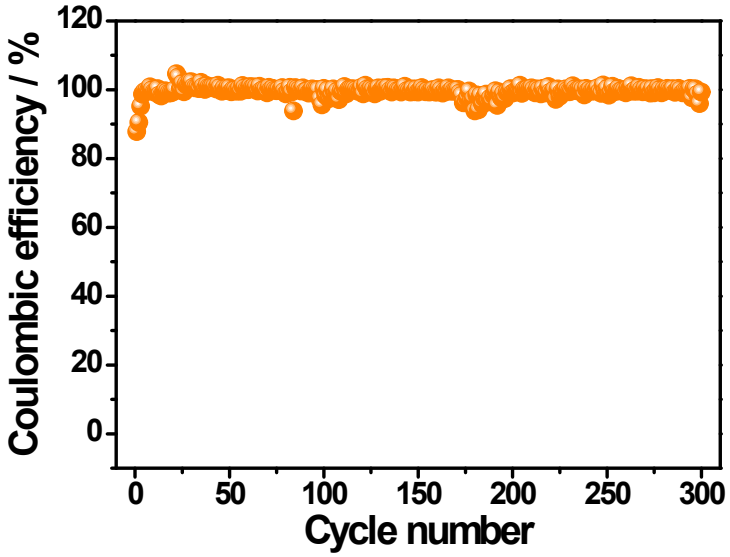


**Fig. S7** The Coulombic efficiency of the assembled dual-ion battery based on activated $NbSe_2$ anode and graphite cathode.

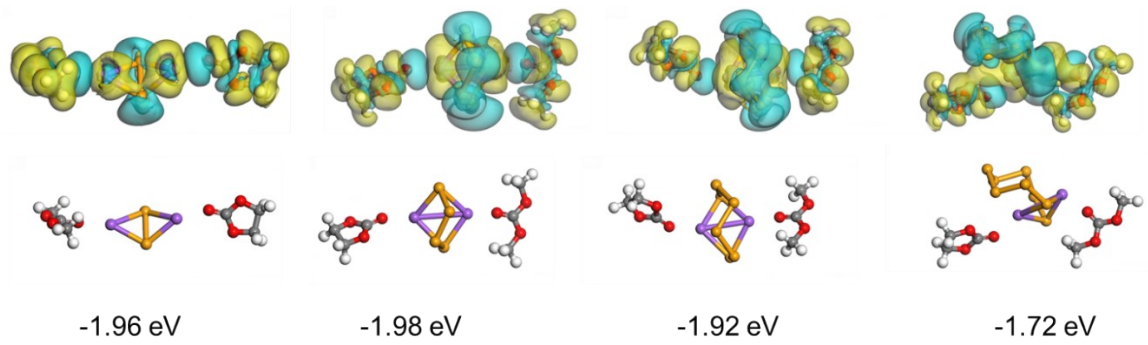


**Fig. S8** The calculated dissolution energy of intermediate $Na_2Se_x$ species in the used electrolyte solvents.

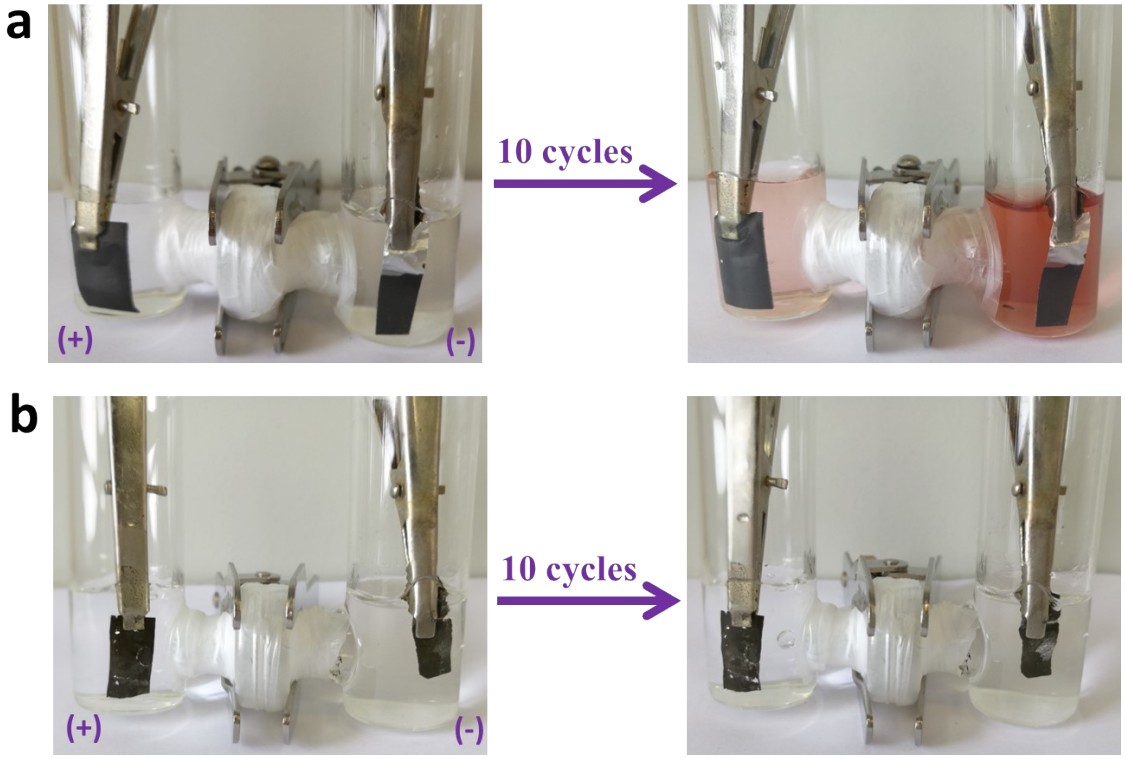


**Fig. S9** Photographs of the dual-ion battery using (a) pure Se and (b) Nb/Se (activated $NbSe_2$) anodes in a two-electrode glass cell device. To understand the inhibition effect of polyselenides, two-electrode glass battery device was assembled to observe the dissolution behavior during charge/discharge process.

**Table S1.** Main electrochemical performance parameters of $NbSe_2$ based electrodes in half-cell tests.

| Electrodes | Stored metal ion | Maximum reversible capacity / mAh $g^{-1}$ | Cycle/capacity retention | Ref. |
|---|---|---|---|---|
| $NbSe_2$ nanosheets | Li-ion | 347 | - | 1 |
| $NbSe_2$ nanoparticles | Li-ion | 313 | - | 2 |
| | Mg-ion | 101 | 42% after 40 cycles | |
| $NbSe_2$ flakes | K-ion | 115 | 91% after 40 cycles | 3 |
| $NbSe_2$ flakes | Na-ion | ~125 | 84% after 100 cycles | 4 |
| $NbSe_2$ nanoparticles | Na-ion | 154 | 94% after 100 cycles | 5 |
| | Li-ion | 485 | 83% after 100 cycles | |
| $NbSe_2$ / N,Se co-doped CNFs | K-ion | 288 | ~100% after 1200 cycles | 6 |
| $NbSe_2$@graphene | Li-ion | 489 | >100% after 1000 cycles | 7 |
| Flower-like $Nb_2Se_9$ | Li-ion | 672 | 88% after 250 cycles | 8 |
| | Na-ion | 342 | 52% after 250 cycles | |
| $NbSe_2$/SnSe | K-ion | ~375 | ~75% after 1000 cycles | 9 |
| $NbSe_2$/$NbS_2$ | Na-ion | ~200 | 92% after 500 cycles | 10 |
| $NbSe_2$ flakes | Na-ion | 212 | 72% after 500 cycles | This work |

**References**


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