

# Supporting Information

## Preparation of Heavily Doped P-Type PbSe with High Thermoelectric Performance by the NaCl Salt-Assisted Approach

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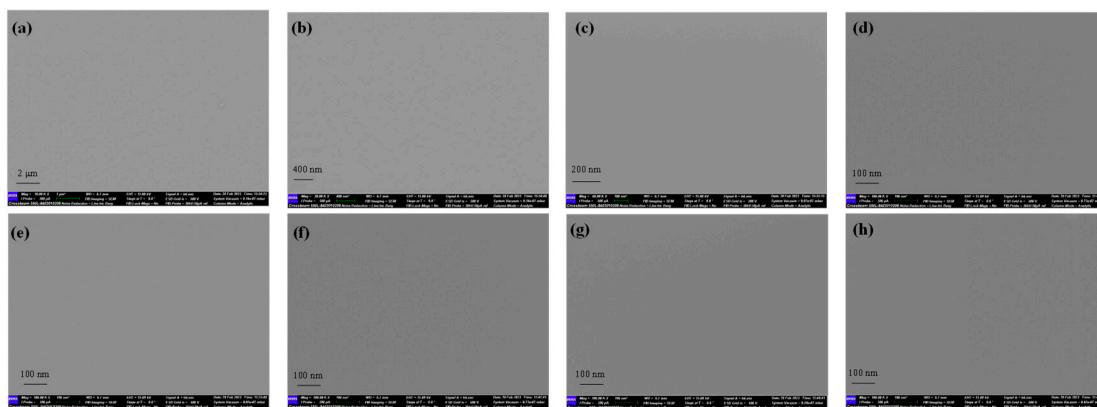
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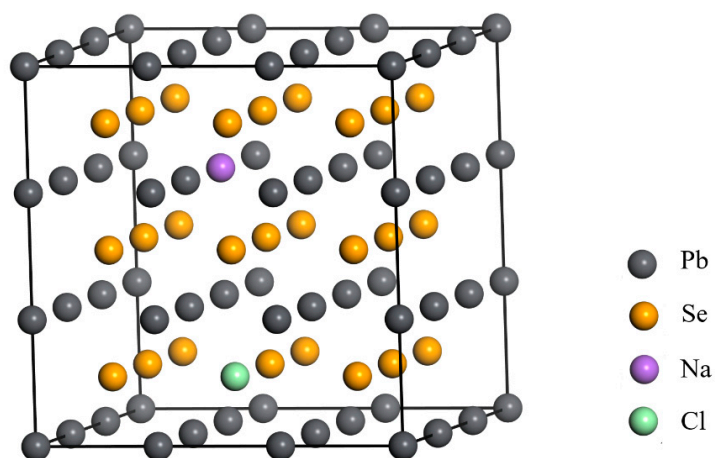
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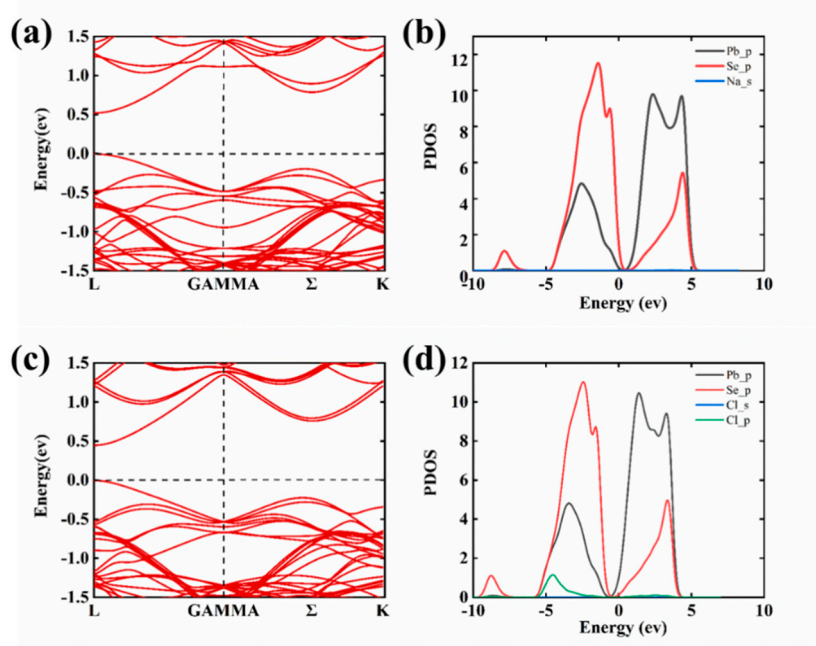
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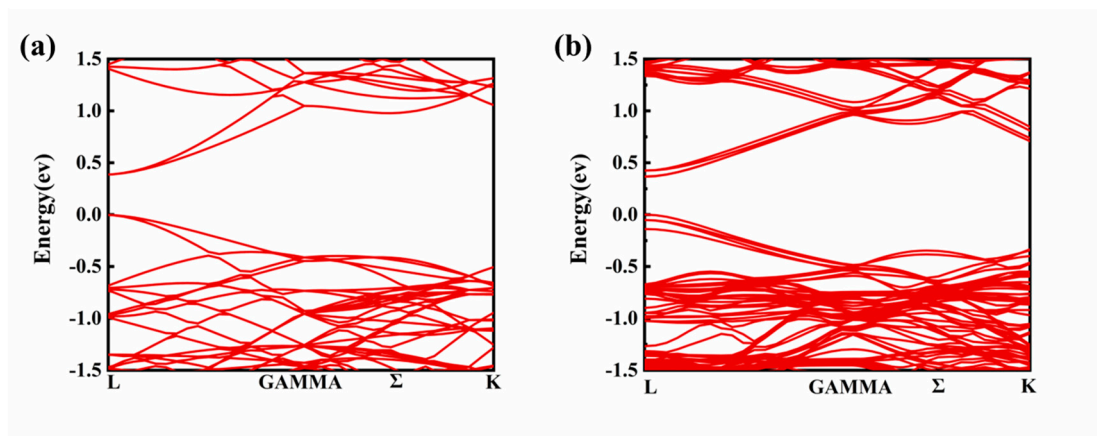
**Figure S1.** FESEM images of  $\text{PbSe}(\text{NaCl})_3$ , which with different magnifications (10000-100000 magnification) (a-d) and from different positions at 100000 magnification (e-h).



**Figure S2.** The crystal structure of  $\text{PbSe}$  doped with only one atom in each species.



**Figure S3.** Band structure and DOS calculated using the  $3\times 3\times 3$  supercell. Band structure of Na-doped PbSe with  $\Delta E_v \sim 0.18$  eV (a); Cl-doped PbSe with  $\Delta E_v \sim 0.22$  eV (c); and corresponding density of states with only one atom substitution for Na-doped PbSe (b); and Cl-doped PbSe (d), where the corresponding states are displayed to clearly show their contribution.



**Figure S4.** Band structure calculated using the  $4\times 4\times 4$  supercell. Band structure of PbSe with  $\Delta E_v \sim 0.42$  eV (a); NaCl-doped PbSe with  $\Delta E_v \sim 0.33$  eV (b).