Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides

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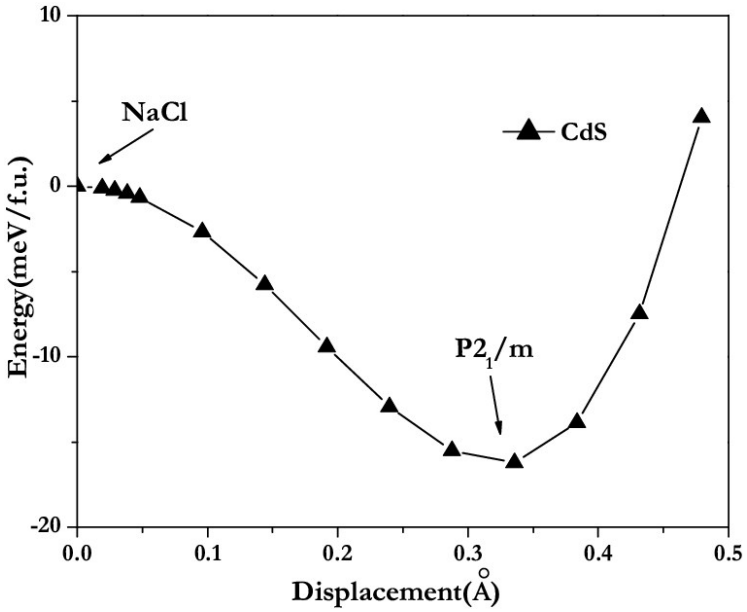

Figure S1. The corresponding energy evolution related to phase transitions of *NaCl*→*P*2$_1$/*m* CdS with the relevant atom displacement (see Figure 2b).

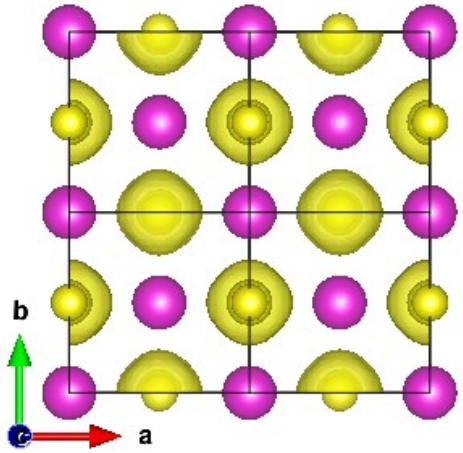

Figure S2. The calculated electron localization functions (ELF) of tetragonal *P*4/*nmm* (*Z* = 2) phase for CdS at 120 GPa. The isosurface value is set as 0.75. The S atoms are small and yellow and the Cd atoms are large and pink.

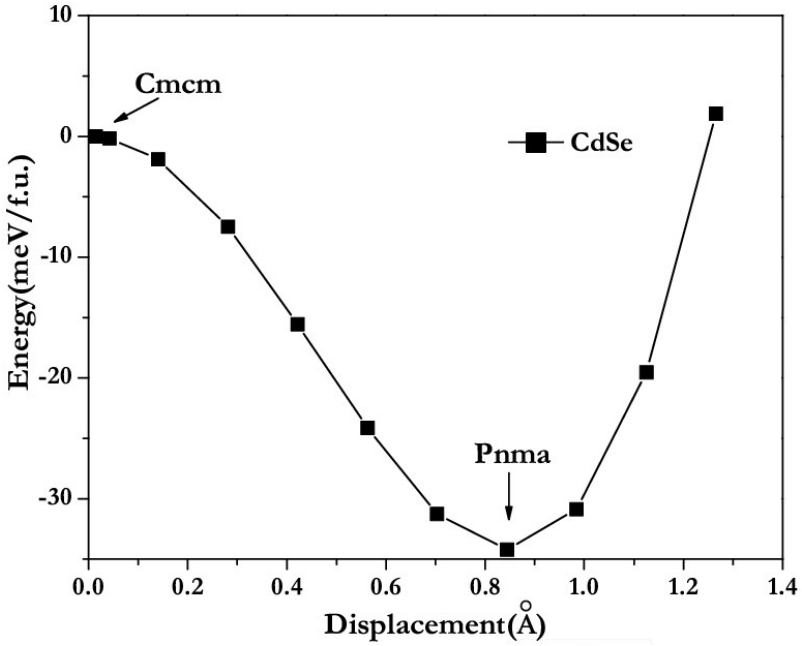

Figure S3. The corresponding energy evolution related to phase transitions of *Cmcm*→*Pnma* CdSe with the relevant atom displacement (see Figure 2d).

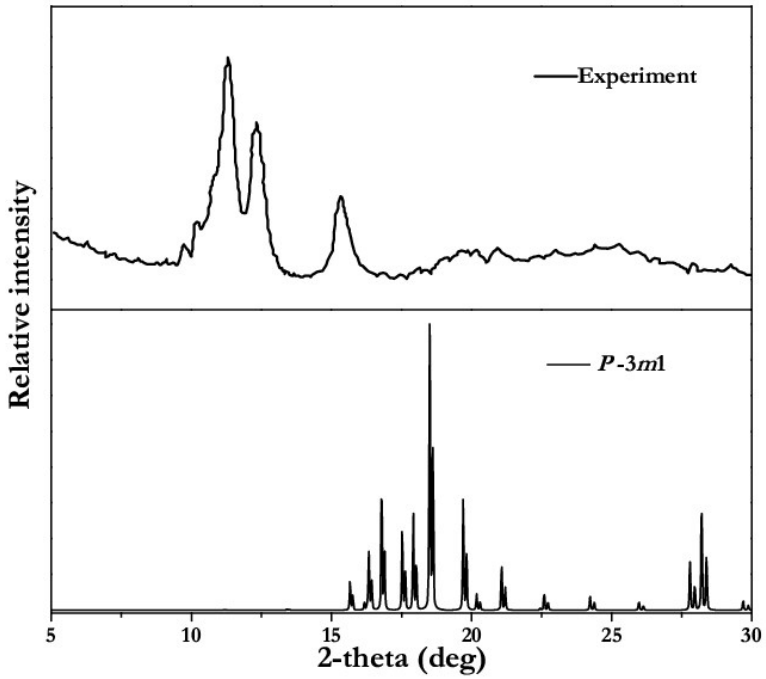

Figure S4. The simulated x-ray diffraction patterns for the metastable *P*-3*m*1 phase of CdTe compared with the experimental data for the unresolved phase at 55 GPa.