

Supplementary Materials

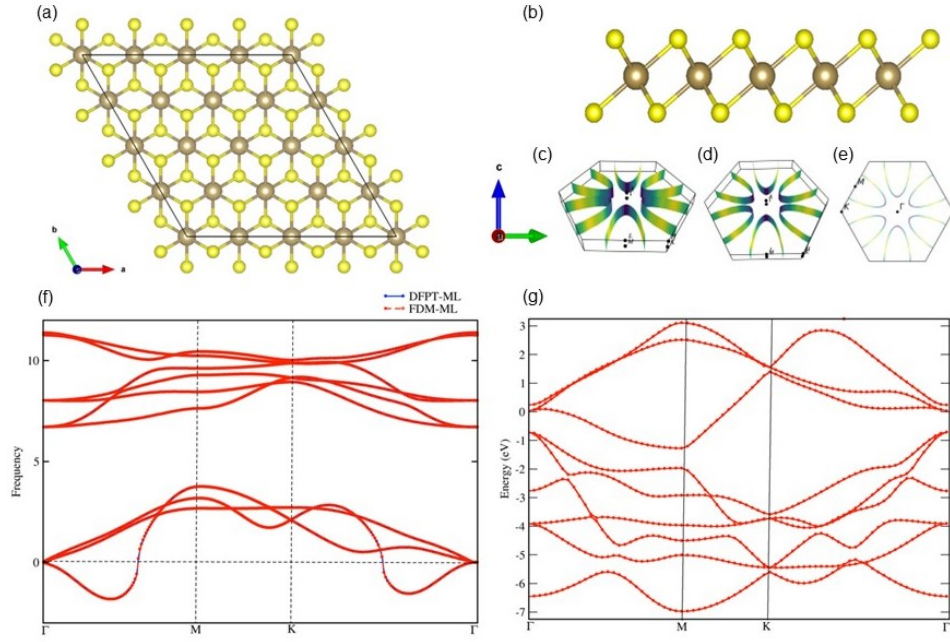


Figure S1: Atomic structures of a 1T-TaS₂ monolayer (a) top view and (b) side way. (c-e) shows the Fermi surface from side view, top view and slice view of the monolayer phase. (f) phonon dispersion plot showing soft phonon modes as negative frequencies. (g) the electronic band structure along high symmetry directions.

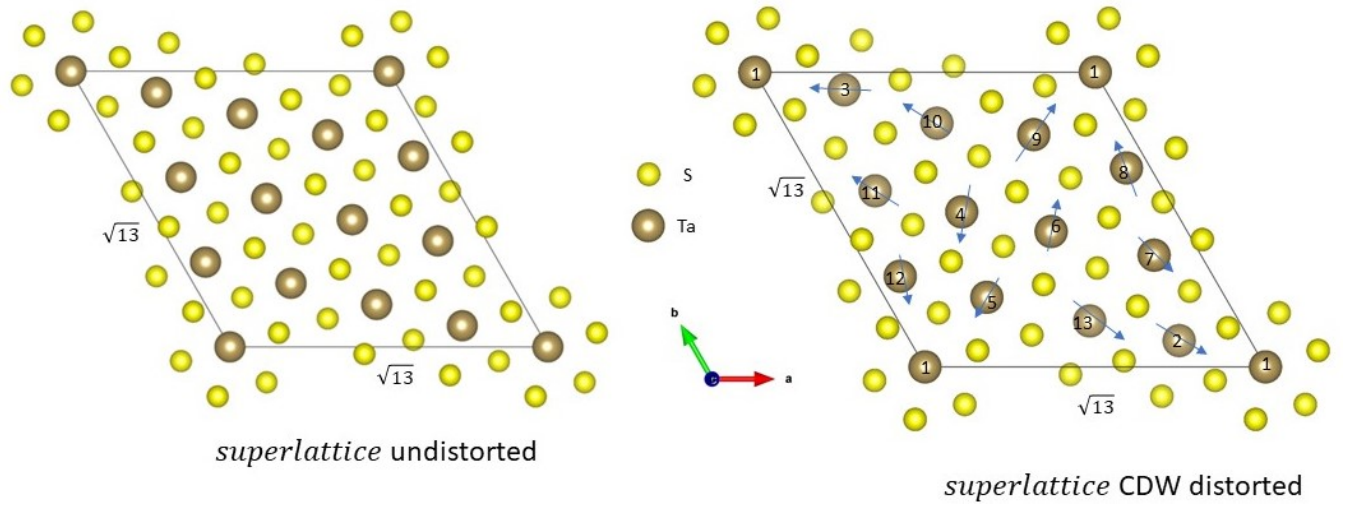


Figure S2: Periodic lattice distortion to obtain CCDW phase from the undistorted superlattice phase.

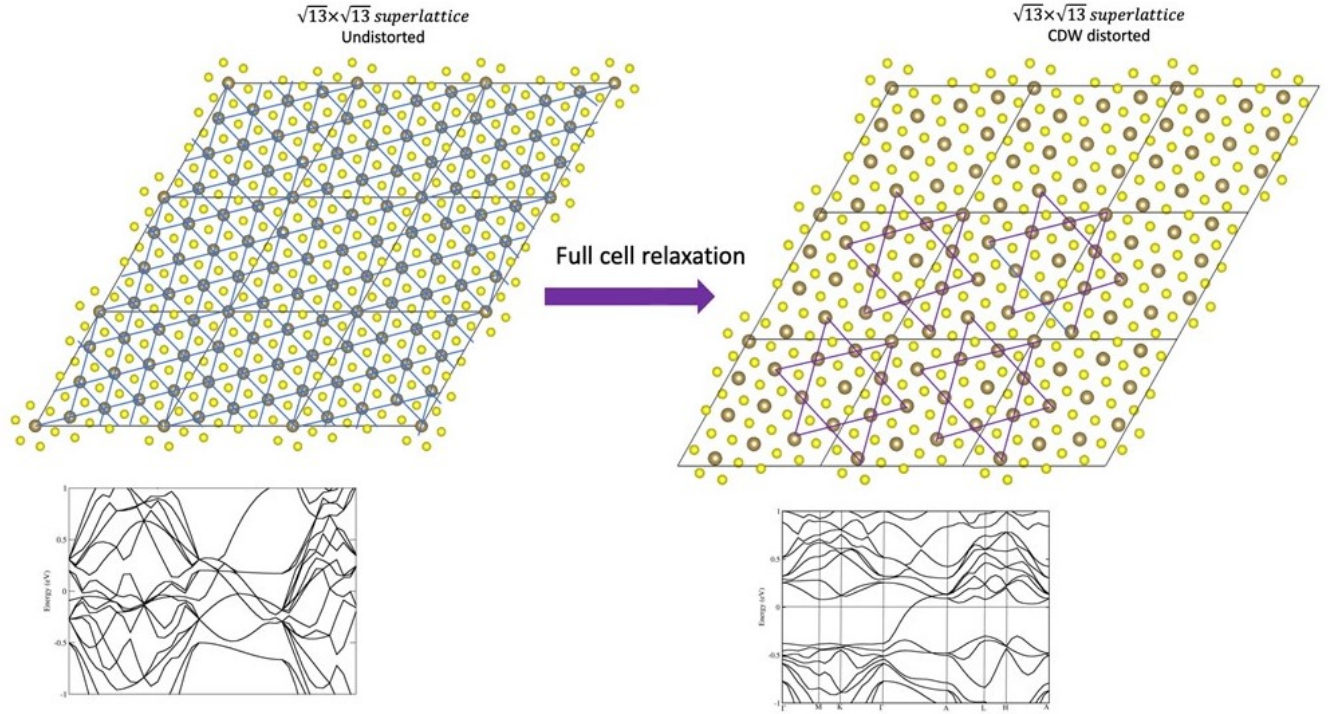


Figure S3: Lattice relaxation for bulk CCDW phase with electronic band structure plots.

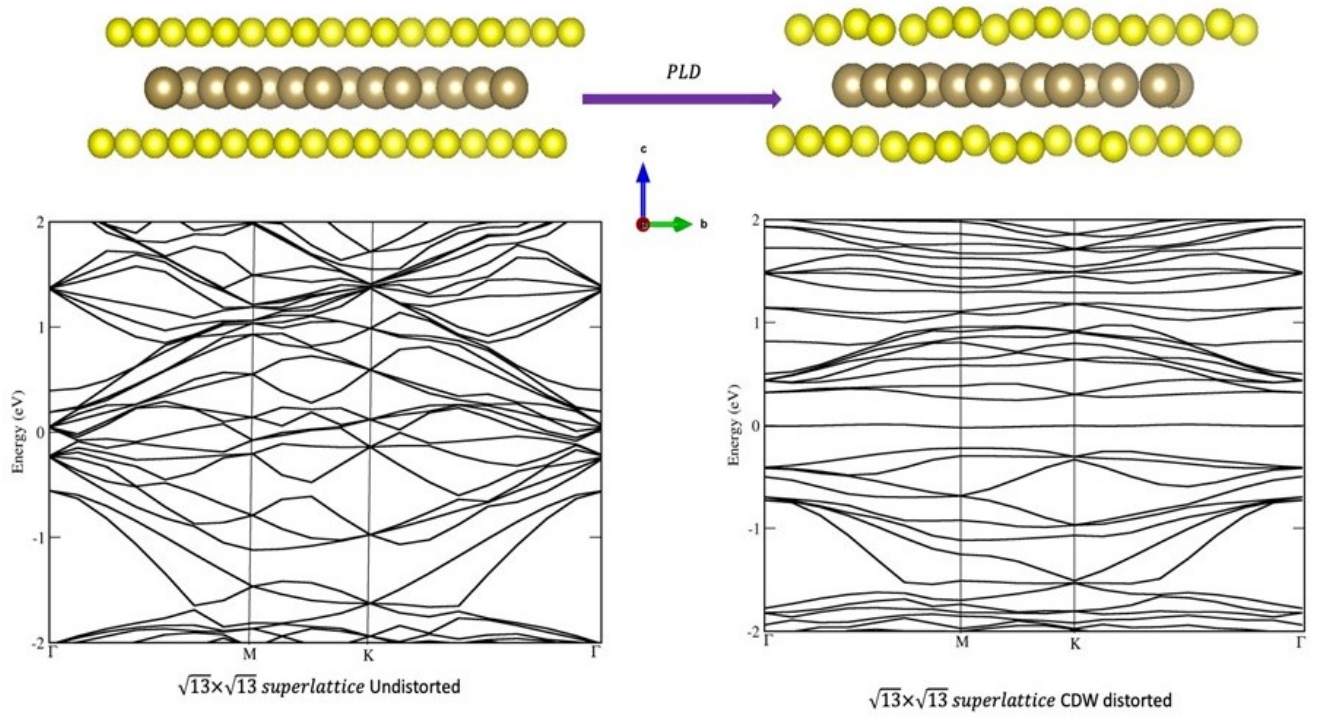


Figure S4: Lattice relaxation for monolayer CCDW phase with electronic band structure plots.