

Description of additional supplementary files

Supplementary Data file: This Supplementary Data zip file contains a text file in the json format which contains the input settings for all DFT calculations, the optimized geometry and the resulting energy. The file can be read by any text editor or by the Atomic Simulation Environment (ASE) database (<https://wiki.fysik.dtu.dk/ase/ase/db/db.html>) module.