

The following files are available for

The dynamics of stacking in layered covalent organic frameworks

as submitted to

Monatshefte der Chemie – Chemical Monthly

Animations:

- **4-layer_system_run_1_0.5ns_MD_trajectory.mp4**
An animation video of a 4-layer system of COF-1 during a 0.5 ns MD run. This corresponds to “run 1” as described in Table 1 the publication.
- **supercell_convergence_1x1_1ns_MD_trajectory.mp4**
An animation video of a 2-layer system of COF-1 during a 1 ns MD run. This corresponds to the “1x1” calculation for supercell convergence as described in the publication.
- **supercell_convergence_4x4_1ns_MD_trajectory.mp4**
An animation video of a 2-layer system of COF-1 during a 1 ns MD run. This corresponds to the “4x4” calculation for supercell convergence as described in the publication.

Calculations:

- **0000_build**
Contains input geometry files that serve as a starting point for most calculations.
- **0100_convergence**
Contains 3 sets of DFT calculations for the convergence tests as described in the Supplementary Figure S12 in the SI of the publication.
- **0201_training_static_inc**
Contains FHI-aims geometry optimizations, VASP single point calculations, and the VASP calculations to generate a force field on that training data. Inclined structures only.
- **0202_training_static_ser**
Contains FHI-aims geometry optimizations, VASP single point calculations, and the VASP calculations to generate a force field on that training data. Serrated structures only.
- **0203_select**
Contains the VASP select calculation, that generates a force field out of a set of training calculations.
- **0204_refit**
Contains the VASP refit calculation, that refits the previously obtained force field.
- **0205_validate_inc**
Contains VASP ML_FF single point calculations on the 55 inclined geometries, to validate the inclined PES
- **0206_validate_ser**
Contains VASP ML_FF single point calculations on the 55 serrated geometries, to validate the serrated PES
- **0207_training_AL_I**
Contains all calculations for the second step (active learning) in training the force field as described in the publication.
- **0208_validate_inc**
Contains VASP ML_FF single point calculations on the 55 inclined geometries, to validate the inclined PES
- **0209_validate_ser**
Contains VASP ML_FF single point calculations on the 55 serrated geometries, to validate the serrated PES
- **0210_training_AL**
Contains all calculations for the third step (active learning) in training the force field as described in the publication.

- **0211_select**
Contains the VASP select calculation, that generates a force field out of a set of training calculations.
- **0212_refit**
Contains the VASP refit calculation, that refits the previously obtained force field.
- **0213_validate_inc**
Contains VASP ML_FF single point calculations on the 55 inclined geometries, to validate the inclined PES
- **0214_validate_ser**
Contains VASP ML_FF single point calculations on the 55 serrated geometries, to validate the serrated PES
- **0300_supercell_convergence**
Contains the 6 MD runs for supercell convergence as described in the publication.
- **0400_minima_stability**
Contains 3 sets of 5 MD runs with different initial geometries, to test the stability of certain energy minima, as described in the publication.
- **0500_thermal_expansion**
Contains the 6 MD runs at fixed temperature from 100 K to 600 K from which the thermal expansion coefficients in the publication have been deduced.
- **0600_4_layers**
Contains the 5 MD runs of COF-1 systems with 4 layers with different initial geometries, as described in the publication.