Simulation data for *Investigating the quasi-liquid layer on ice surfaces: a comparison of order parameters*

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Data for cubic ice (Ic), hexagonal ice (Ih) and supercooled water (wIh) in bulk systems, and Ic-(001) plane, Ih-basal plane, Ih-primary prismatic (prism1) plane, and Ih-secondary prismatic (prism2) plane in surface slab systems. These data are relative to molecular dynamics (MD) simulations performed with LAMMPS (Dec 9, 2014 version) package and to analysis with PLUMED 2.5.1.

The TIP4P/Ice water potential was used for the simulations.

The data are divided into tiers of files. Each tier's files are characterised by one or more labels, which are mentioned here where appropriate.

MD input and data files for bulk and surface systems

Compressed folders:

- *Bulk_MD_Model_Inp.tar.gz:* data and LAMMPS input files for bulk
- *Surf_MD_Model_Inp.tar.gz:* data and LAMMPS input files for surface

Structure names:

- *data.2744Ic:* data file for bulk-Ic containing 2744 molecules
- *data.2880Ih:* data file for bulk-Ih, bulk-wIh containing 2880 molecules
- *data.5488Ic:* data file for surface-Ic containing 5488 molecules
- *5760_basalz_oxy.xyz:* coordinates file for the Ih-basal model
- *5760_prism1y_oxy.xyz:* coordinates file for the Ih-prism1 model
- *5760_prism2x_oxy.xyz:* coordinates file for the Ih-prism2 model

LAMMPS input names:

- *NPT*:* NPT equilibration
- *NVT*:* NVT production

Cell dimensions after final NVT run:

- *cell_data-temp-basal.dat:* cell size for basal
- *cell_data-temp-prism1.dat:* cell size for prism1
- *cell_data-temp-prism2.dat:* cell size for prism2

MD trajectories for bulk and surface systems

Compressed folders:

- *Bulk_MD_Tra.tar.gz:* trajectories files for bulk
- *Surf_MD_Tra.tar.gz:* trajectories files for surface

Bulk system:

- *oxy:* trajectory for only oxygen atoms

Surface system:

- *TALL100ns:* trajectory of all 100 ns NVT
- *oxy:* trajectory for only oxygen atoms

PLUMED data file and analysis results of bulk system

Compressed folders:

- *BulkIc_PLUMED.tar.gz:* data file and analysis results for bulk-Ic
- *BulkIh_PLUMED.tar.gz:* data file and analysis results for bulk-Ih

Bulk-Ic and bulk-Ih:

- *250 K, 260 K:* relevant temperatures
- *histo:* histogram of the relevant order parameter
- *q3, q4, q6:* global Steinhardt order parameters
- *lq3, lq4, lq6:* local Steinhardt order parameters
- *laq3, laq4, laq6:* local averaged Steinhardt order parameters
- *entropy, localentropy:* entropy fingerprint and local-averaged entropy fingerprint
- *xyz:* coordinates of atoms and the respective value of the collective variables
- *plumed*.dat:* PLUMED data files

PLUMED data file and analysis results of surface system

Compressed folders:

- *SurfIc_PLUMED.tar.gz:* analysis results for surface-Ic
- *SurfIh_PLUMED.tar.gz:* analysis results for surface-Ih

Surface-Ic and surface-Ih:

- *lq3, laq3, localentropy:* local and local-averaged Steinhardt order parameters and local-average entropy fingerprint