Supplementary Information (SI) for Nanoscale.


The provided "azopc.tar" archive contains all the files needed to run MD simulations using NAMD. The contents of this archive can be extracted using the command: tar -xvf azopc.tar.

The azo-PC unit cell contains 64 lipids per leaflet for a total of 128 lipids and TIP3P water.

Flies contained in azopc.tar

namdinput_cis_azopc.conf: Configuration file for the pure cis solvated bilayer
namdinput_trans_azopc.conf: Configuration file for the pure trans solvated bilayer
azopc_sol.psf: Protein structure file for the azo-PC bilayer unit cell
trans_azopc_sol_eq.pdb: Equilibrated structure of the pure trans solvated bilayer in PDB format
cis_azopc_sol_eq.pdb: Equilibrated structure of the pure cis solvated bilayer in PDB format
azopc.pdb: Atomic coordinates for a single azo-PC lipid molecule in PDB format
top_C36_azoPC_lipid.rtf: Topology file defining connectivity, atom types, and partial charges for azo-PC lipid
cis.phenol.conf: Configuration file for one molecule of phenol in a cis bilayer system
cis.phenol.pdb: PDB file for one molecule of phenol in a cis bilayer system
cis.phenol.psf: PSF file for one molecule of phenol in a cis bilayer system
trans.phenol.conf: Configuration file for one molecule of phenol in a trans bilayer system
trans.phenol.pdb: PDB file for one molecule of phenol in a trans bilayer system
trans.phenol.psf: PSF file for one molecule of phenol in a trans bilayer system
cis.skf.conf: Configuration file for one molecule of skf in a cis bilayer system
cis.skf.pdb: PDB file for one molecule of skf in a cis bilayer system
cis.skf.psf: PSF file for one molecule of skf in a cis bilayer system
trans.skf.conf: Configuration file for one molecule of skf in a trans bilayer system
trans.skf.pdb: PDB file for one molecule of skf in a trans bilayer system
trans.skf.psf: PSF file for one molecule of skf in a trans bilayer system
Common folder: Force field parameter files