

Breakout session: Soft matter

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LAMMPS resources for soft matter

- **Manual**

- Section 6.3 = CHARMM, AMBER, Dreiding ff
- Section 6.7 = TIP3P water
- Section 6.8 = TIP4P water
- Section 6.9 = SPC water
- Section 6.21 = viscosity
- Section 6.22 = diffusion constants
- Section 6.26 = Drude induced dipoles

- **Pair styles**

- pair: morse, charmm, class2, lj/coul, nm, tip4p
- reactive: reax/c (omp,kokkos)
- kim = <https://openkim.org>

- **Fixes**

- cmap, evaporate, shake, viscosity, viscous

LAMMPS resources (continued)

- **Computes**
 - gyration, msd
- **Packages**
 - CLASS2, DIPOLE, MANYBODY, MOLECULE, COLLOID, USER-SPH, DRUDE, USER-COLVARS
- **Example dirs**
 - cmap, colloid, flow, melt, obstacle, peptide, DIFFUSE, VISCOSITY