

# **Breakout Session: Interfaces (solid/liquid)**

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# System details

## Types of interfaces

Solid-gas  
Solid-Solid  
Liquid-Gas  
Liquid-Liquid  
**Solid-Liquid**

## Properties to be simulated

Structure  
Transport  
Spectroscopic

## Interaction potentials

Atomistic  
Coarse-grained  
Same pair style for both phases (hopefully)  
Hybrid pair style

# LAMMPS resources for interfaces

See breakout resource pages for **solid-state** and **soft matter**

## Pair styles

- pair hybrid
- pair hybrid/overlay

## Solid-state pair styles

- pairwise: born, buckingham, morse
- many-body: eam, edip, eim, gw, mgpt, sw, terso, meam, nb3b, polymorphic, rebo, airebo, snap, sw, terso, vashishita
- reactive: comb, comb3, reax/c (omp, kokkos)
- kim = <https://openkim.org> pair hybrid/overlay

## Soft matter pair styles

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

# Pre- and post-processing

## Pre-processing

- Initial configuration
- Choice of FF, boundary conditions
- Solid phase – fixed atoms or mobile/flexible

## Post-processing

- Not the same as bulk phases
- Calculation of properties as a function of distance from the interface