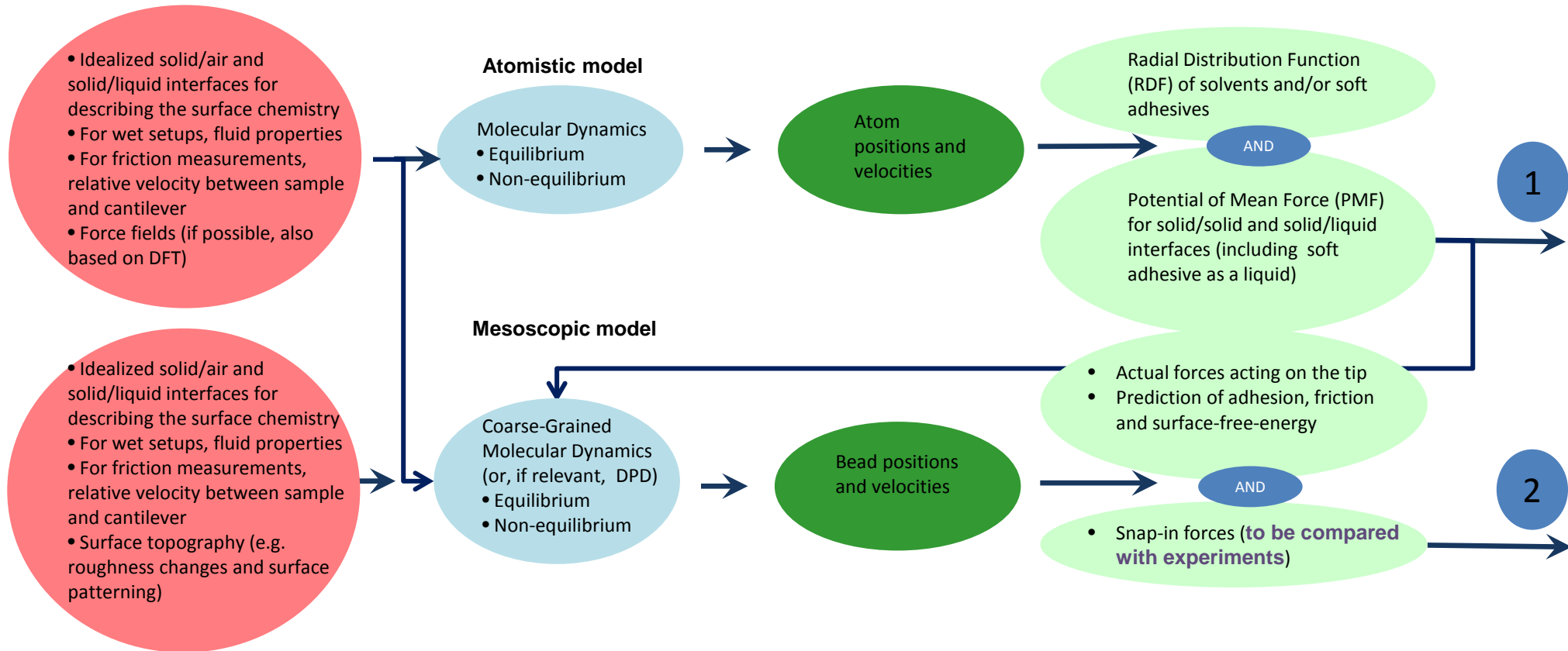


# Workflow for modelling Adhesion (A) and Surface-Free-Energy (SFE): effects in coatings and composites



# Workflow for modelling Adhesion (A) and Surface-Free-Energy (SFE): effects in coatings and composites

1

- Idealized solid/air and solid/liquid interfaces for describing the surface chemistry
- Surface topography (e.g. roughness changes and surface patterning)
- Droplet fluid properties

## Mesoscopic model

Coarse-Grained Molecular Dynamics (or, if relevant, DPD)

- Equilibrium
- Non-equilibrium

Bead positions and velocities

Prediction of contact angle of droplets and hydrophobicity / hydrophilicity of surfaces

## Continuum model

Droplet fluid mechanics on surfaces

Velocity and temperature

Prediction of contact angle of droplets and hydrophobicity / hydrophilicity of surfaces **(to be compared with experiments)**

2

New theory(?) correlating snap-in forces with hydrophobicity / hydrophilicity

Measurement #3:  
Contact angles

Validation and interpretation of experiments

OYSTER #760827