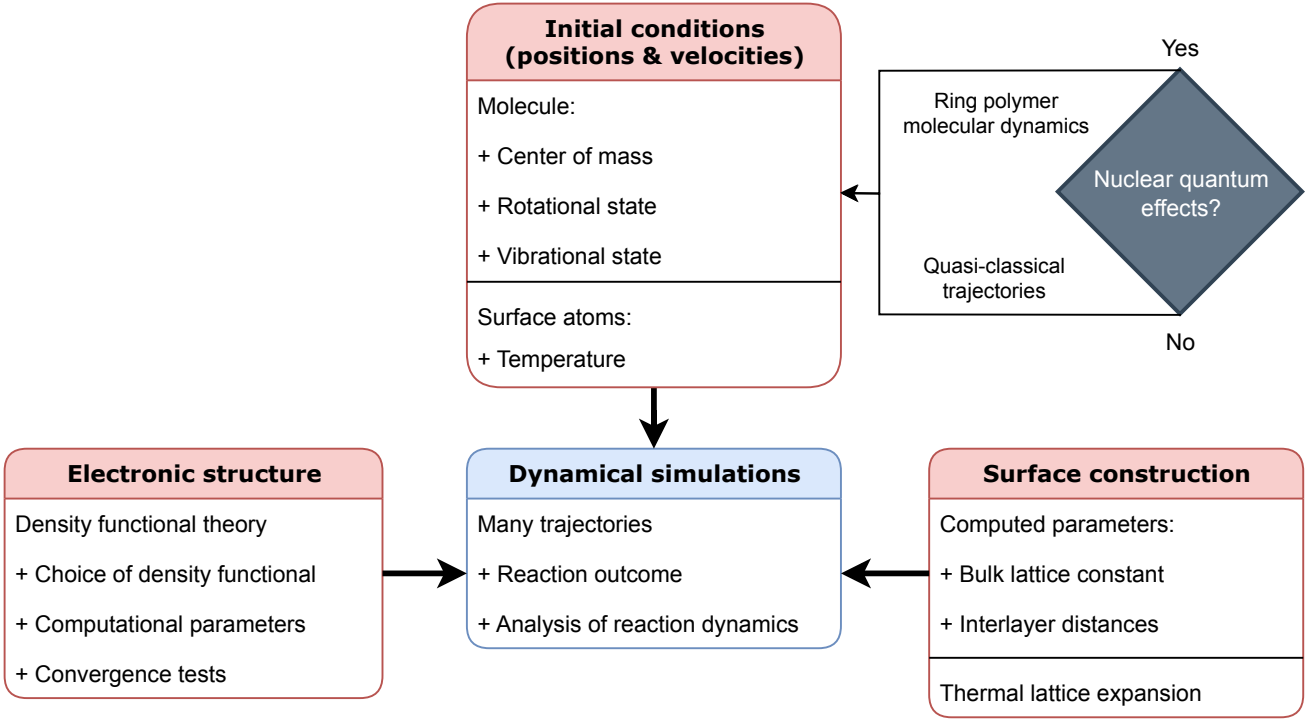
Initial conditions (positions & velocities)
Molecule:
+ Center of mass
+ Rotational state
+ Vibrational state
Surface atoms:
+ Temperature
Yes
Ring polymer molecular dynamics
Nuclear quantum effects?
Quasi-classical trajectories
No
Electronic structure
Density functional theory
+ Choice of density functional
+ Computational parameters
+ Convergence tests
Dynamical simulations
Many trajectories
+ Reaction outcome
+ Analysis of reaction dynamics
Surface construction
Computed parameters:
+ Bulk lattice constant
+ Interlayer distances
Thermal lattice expansion