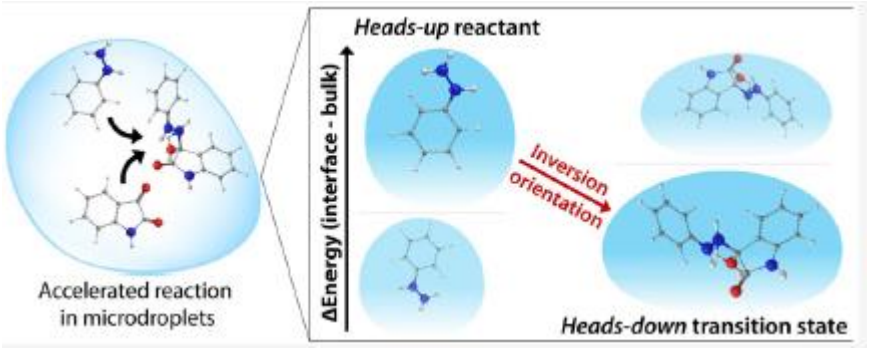
Quantum modeling of reactions in microdroplets

Motivation:

Reaction acceleration (up to 10^6) observed in microdroplets

Objective:

- ❑ Explicit solvent calculation (~1400 atoms) at microdroplet/air interface
- ❑ Verify hypothesis of partial solvation at interface



Approach:

- ❑ Gaussian – Reaction pathway
- ❑ DFTB – Solvent calculation

Results:

- ❑ Neutral molecules – Fully solvated at interface
- ❑ Charged molecules – Solvation is dipole orientation dependent