

## SHARC Workflow

Preparation

Optimization

$\mathbf{R}_{\text{eq}}$

Frequencies

$\mathbf{R}_{\text{eq}}, \{\nu_i\}, \{\mathbf{n}_i\}$

Wigner Sampling

$\{(\mathbf{R}, \mathbf{v})_k\}$

Initial Conditions

Setup

Excited-State Calcs.

$\{\Delta E_{k,\beta}\}, \{F_{k,\beta}^{\text{osc}}\}$

Excited-State Selection

$\{(\mathbf{R}, \mathbf{v}, \alpha)_k\}$

Setup

Dynamics

Analysis

Aftermath

Quantum Chemistry

Quantum Chemistry

freq.molden

wigner.py

initconds

setup\_init.py

Quantum Chemistry

QM.out

excite.py

initconds.excited

setup\_traj.py

sharc.x

output.dat, output.xyz

many tools...