Supporting Information **NEXMD Software Package for Non-adiabatic Excited State Molecular Dynamics Simulations**

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Table S 1: NEXMD output files generated at each verbosity level for each functionality. ◊ denotes an output file that is only generated for an excited state calculation.

Verbosity	File	Geometry Optimization (GS or ES)	Single Point (GS or ES)	Adiabatic BOMD (GS or ES)	NAMD
0	coefficient.out	◊			X
	coords.xyz	X	X	X	X
	energy-ev.out	X	X	X	X
	restart.out			X	X
	hops.out				X
	temperature.out			X	X
	velocity.out	X	X	X	X
1	coeff-n.out	◊			X
	nacr.out				X
	nact.out				X
	pes.out	◊	◊	◊	X
	transition-densities.out	◊	◊	◊	X
2	cross-steps.out				X
	hops-trial.out				X
	order.out				X
3	cm.out	X	X	X	X
	coeff-q.out				X
	forces.out	X	X	X	X

Table S 2: Description of each file written for different NEXMD verbosity levels.

Verbosity	File	Description
0	coefficient.out	quantum populations (unitless)
	coords.xyz	atomic cartesian coordinates (Å)
	energy-ev.out	kinetic energy (eV), potential energy (eV), total energy (eV), and their respective changes from t=0 (eV)
	restart.out	coordinates (Å), velocity (Å/ps), quantum coefficients and phases, current state, current time, and random seed at the last time step
	hops.out	hop type, state before hop, state after hop, total energy before hop (Hartrees), total energy after hop (Hartrees)
	temperature.out	temperature (K), temperature of thermostat (K)
	velocity.out	velocity (XYZ) of each atom (Å/ps)
1	coeff-n.out	current state, quantum coefficients of all states, and their sum (unitless)
	nacr.out	nonadiabatic coupling vector for each atom (1/Å)
	nact.out	nonadiabatic coupling scalar between each state (1/ps)
	pes.out	potential energy of each adiabatic state (eV)
	transition-densities.out	diagonal elements of the transition density for each atomic orbital in the current state (unitless)
2	cross-steps.out	overlap of states that may cross (unitless)
	hops-trial.out	lists of all attempted hops and states involved
	order.out	order of adiabatic states with respect to the initial ordering at t=0
3	cm.out	coordinates of the center of mass with respect to t=0 (Å)
	coeff-q.out	phase of each quantum coefficient
	forces.out	forces (XYZ) on each atom (eV/Å)