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Supporting Information for

Non-Adiabatic Excited State Molecular Dynamics Methodologies:

Comparison and Convergence

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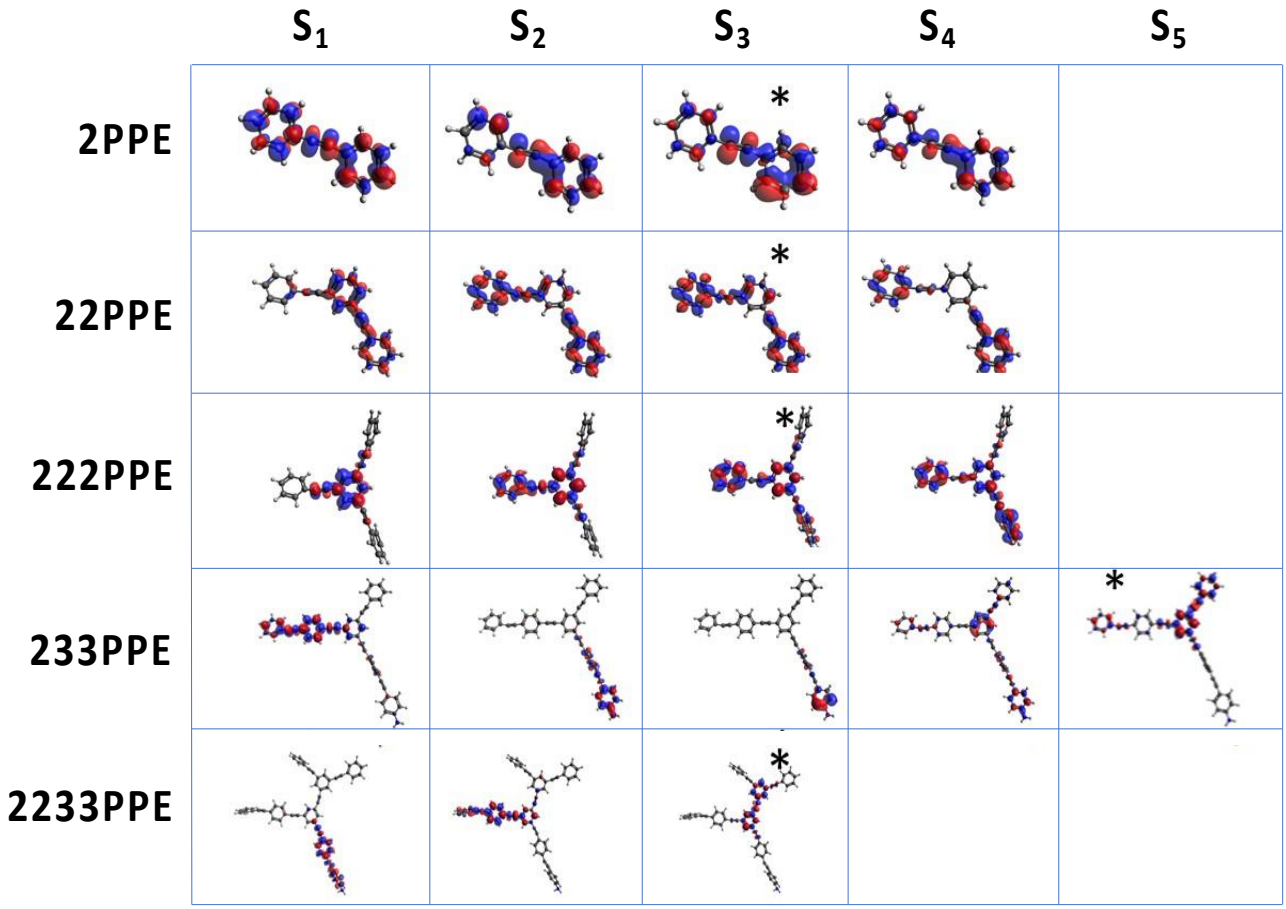

Figure S1. Localization of electronic transition densities for the excited states considered in our simulations for a random initial configuration from the 300 K conformational sampling. The asterisk marks the initial state for excited state dynamics.

Table S1. AIMC parameters used to generate data presented in **Figure 5**.

Molecule	panel	Number of initial conditions	δ_2(cloning criteria)	Maximum number of cloning events allowed	Gaussian widths	Total number of cloning events
2PPE	a)	**100**	5°	16	α	980
2PPE	a)	**200**	5°	16	α	2550
2PPE	a)	**300**	5°	16	α	4110
2PPE	a)	**400**	5°	16	α	5676
2PPE	a)	**500**	5°	16	α	7269
2PPE	a)	**600**	5°	16	α	8822

222PPE	b)	**100**	5°	16	α	1072
222PPE	b)	**200**	5°	16	α	2750
222PPE	b)	**300**	5°	16	α	4312
222PPE	b)	**400**	5°	16	α	6065
222PPE	b)	**500**	5°	16	α	7728
222PPE	b)	**600**	5°	16	α	9376
2PPE	c)	300	15°	16	α	**2942**
2PPE	c)	300	10°	16	α	**3674**
2PPE	c)	300	5°	16	α	**4110**
2PPE	c)	300	1°	16	α	**4162**
2PPE	c)	300	5°	32	α	**7936**
2PPE	c)	300	1°	32	α	**8070**
222PPE	d)	300	15°	16	α	**3077**
222PPE	d)	300	10°	16	α	**4098**
222PPE	d)	300	5°	16	α	**4312**
222PPE	d)	300	1°	16	α	**4346**
222PPE	d)	300	5°	32	α	**8954**
222PPE	d)	300	1°	32	α	**9087**
2PPE	e)	300	5°	16	$\mathbf{0}\,\boldsymbol{\alpha}$	4110
2PPE	e)	300	5°	16	$\mathbf{0.5}\boldsymbol{\alpha}$	4110
2PPE	e)	300	5°	16	$\boldsymbol{\alpha}$	4110
2PPE	e)	300	5°	16	$\mathbf{2}\boldsymbol{\alpha}$	4312
222PPE	f)	300	5°	16	$\mathbf{0}\,\boldsymbol{\alpha}$	4312
222PPE	f)	300	5°	16	$\mathbf{0.5}\boldsymbol{\alpha}$	4312
222PPE	f)	300	5°	16	$\boldsymbol{\alpha}$	4312
222PPE	f)	300	5°	16	$\mathbf{2}\boldsymbol{\alpha}$	4312

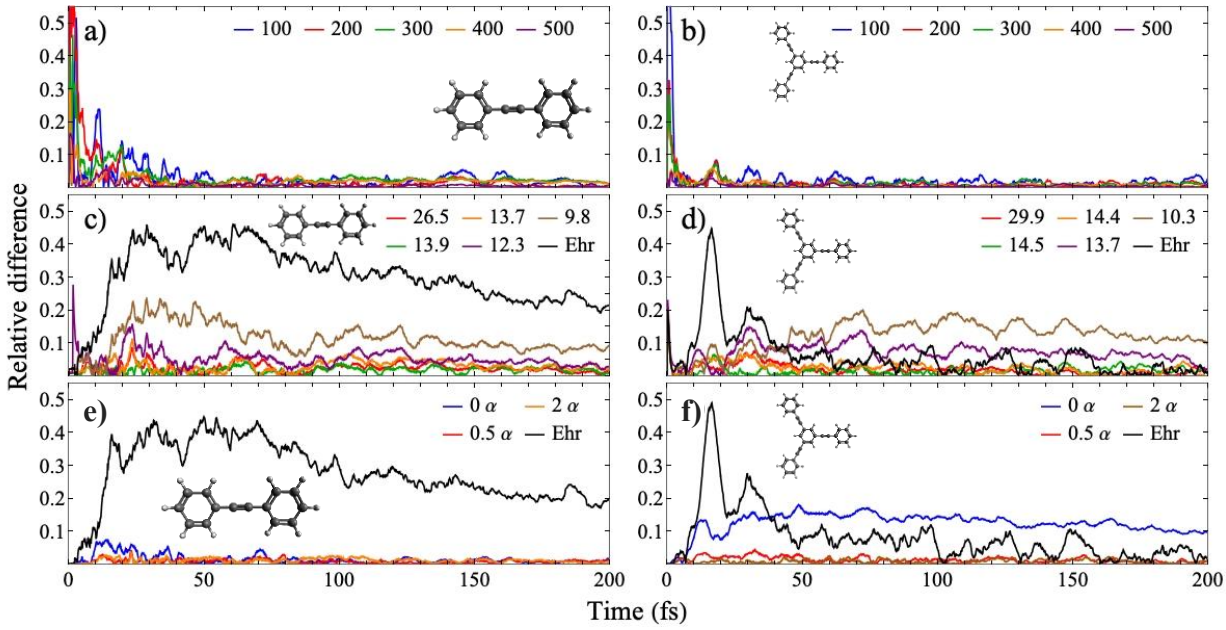

Figure S2. The relative differences between the S_1 adiabatic state populations obtained from EHR and AIMC simulations using different parameters. Relative differences between populations are calculated with respect to our most accurate result as *abs(a-b)/mean(a,b)* where *a* is our tested parameter and *b* is our most accurate result. (a) and (b) Convergence of AIMC results with respect to the number of trajectories for 2PPE and 222PPE, respectively. Relative difference with respect to a 600 trajectory ensemble. (c) and (d) Convergence of AIMC results with respect to the number of cloning events per initial condition for 2PPE and 222PPE, respectively. Relative difference with respect to largest number of cloning events (26.9 for 2PPE and 30.3 for 222PPE). (e) and (f) Analysis of robustness of AIMC results with respect to variations in the α Gaussian width for 2PPE and 222PPE, respectively. Relative error with respect to 1α.