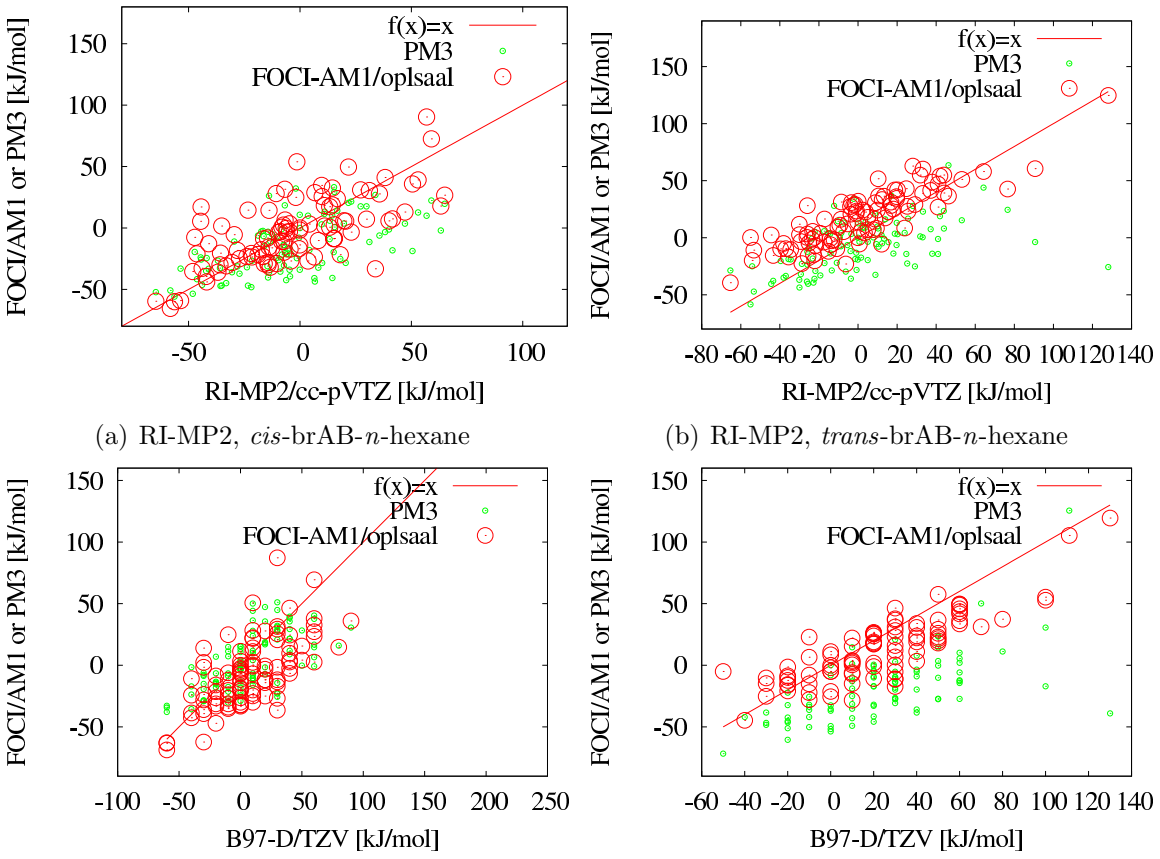
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

QM/MM Surface-Hopping Dynamics of a Bridged Azobenzene Derivative

Electronic Supplementary Information

Correlation plots



(a) RI-MP2, *cis*-brAB-*n*-hexane

(b) RI-MP2, *trans*-brAB-*n*-hexane

(c) B97-D, *cis*-brAB-*n*-hexane

(d) B97-D, *trans*-brAB-*n*-hexane

Figure 1: Correlation plots for benchmark calculations: both PM3 and FOCI-AM1/OPLS-AA energies were plotted against the corresponding RI-MP2 and B97-D energies. AM1 energies were omitted due to clarity.

Simulation results table

Table 1: Simulation results for *cis*→*trans* and *trans*→*cis* photo-isomerization. The listed coordinates are averaged values at the last step(s) on the excited state surface prior to the first surface hop onto the S_0 surface (only counting hops that resulted in stays longer than 25 fs on ground state surface).

cis*→*trans	reactive[a]	unreactive[a]	reactive[b]	unreactive[b]
No. of trajectories	152	98	57	193
Return to S_0 [fs]	129.70	86.79	59.07	45.61
CNNC [Deg]	84.71	81.85	-81.62	-80.45
CNN_1 [Deg]	126.53	129.25	123.27	127.31
CNN_2 [Deg]	123.96	120.65	113.13	114.85
$NNCC_1$ [Deg]	122.30	106.40	102.73	105.38
$NNCC_2$ [Deg]	37.99	23.26	-6.01	-11.47
$CCCC_{Br.}$ [Deg]	57.93	51.00	-41.98	-39.10
dCNNC/dt [Deg/fs]	0.37	0.23	0.51	0.02
$dCCCC_{Br.}$/dt [Deg/fs]	0.15	0.17	0.01	0.04
$dCNN_1$/dt [Deg/fs]	0.17	0.21	0.02	0.33
$dCNN_2$/dt [Deg/fs]	0.15	0.19	0.22	0.15
$dNNCC_1$/dt [Deg/fs]	0.23	0.24	0.35	0.02
$dNNCC_2$/dt [Deg/fs]	0.28	0.30	0.23	0.12
trans*→*cis	reactive[a]	unreactive[a]	reactive[b]	reactive[b]
No. of trajectories	98	152	144	106
Return to S_0 [fs]	29.56	31.59	42.06	41.15
CNNC [Deg]	100.13	99.60	95.95	97.13
$CCCC_{Br.}$ [Deg]	97.89	98.20	107.10	104.85
CNN_1 [Deg]	115.53	115.31	132.96	132.14
CNN_2 [Deg]	114.22	115.04	132.34	132.67
$NNCC_1$ [Deg]	66.83	64.80	-39.94	-41.68
$NNCC_2$ [Deg]	67.34	69.87	-38.46	-40.24
dCNNC/dt [Deg/fs]	0.97	0.93	-0.93	-0.48
$dCCCC_{Br.}$/dt [Deg/fs]	0.20	0.20	0.27	0.25
$dCNN_1$/dt [Deg/fs]	0.29	0.30	0.21	0.13
$dCNN_2$/dt [Deg/fs]	0.31	0.25	0.22	0.13
$dNNCC_1$/dt [Deg/fs]	0.60	0.54	-0.49	-0.24
$dNNCC_2$/dt [Deg/fs]	0.53	0.56	0.48	0.27

[a]QM/MM, this work.
[b]gas phase surface-hopping dynamics (reparametrized FOCI-AM1). [1]

References

[1] Carstensen, O.; Sielk, J.; Schönborn, J.; Granucci, G.; Hartke, B. *J. Chem. Phys.* **2010** *133*, 124305.