

Doubly Tuned Exchange-Correlation Functionals for Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory

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I. MAE AND BOXPLOTS WITH CC-PVTZ BASIS SET

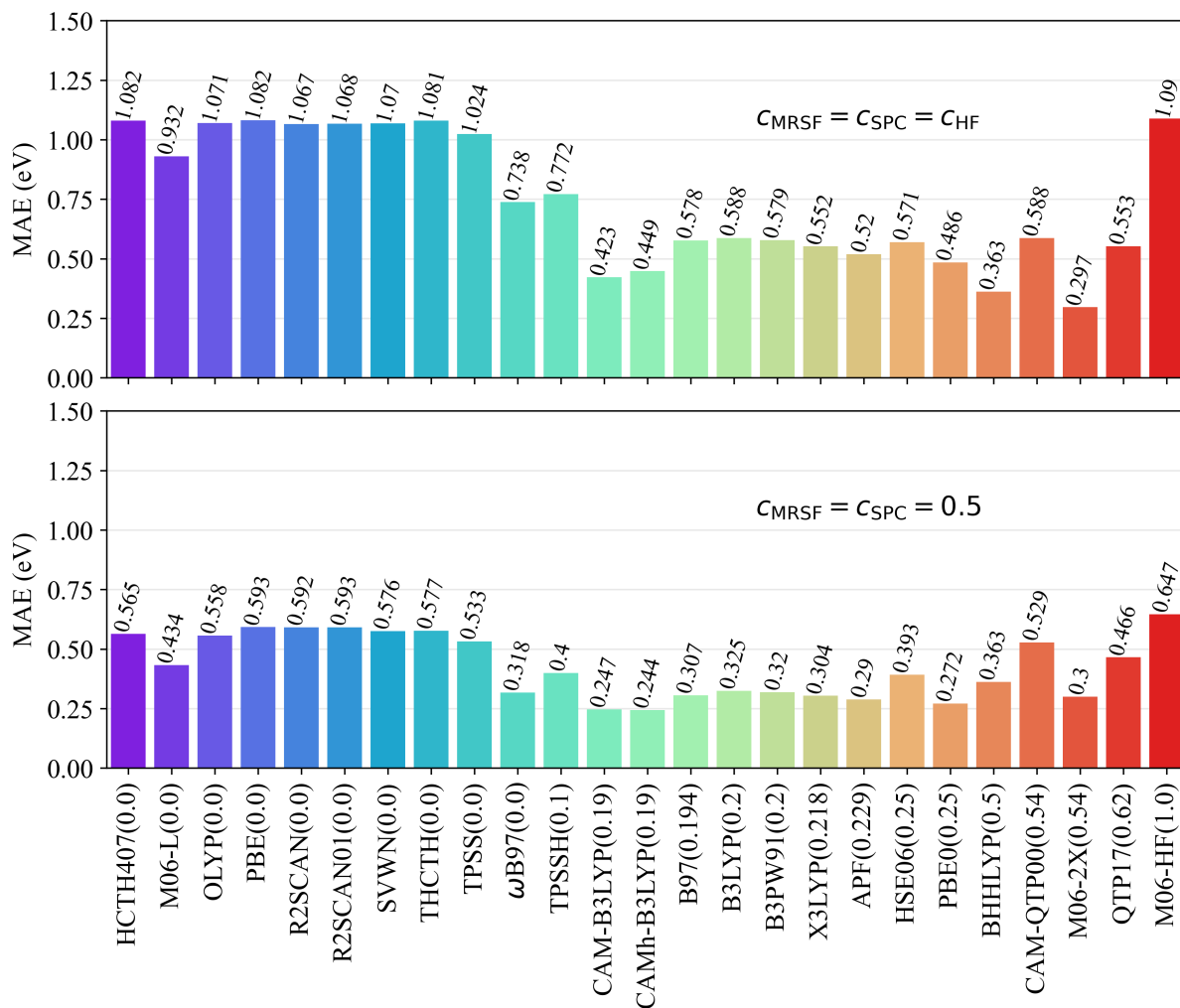


FIG. S1: The mean absolute errors (MAE) (in eV) of S_1 and S_2 excited states against (based on symmetry label of states) the best estimates for Thiel's molecular set as a function of XC functionals, where top figure represents the MAE results with $c_{\text{MRSF}}=c_{\text{SPC}}=c_{\text{HF}}$, while the MAEs of bottom figure were generated with $c_{\text{MRSF}}=c_{\text{SPC}}=0.5$. All calculations were done by MRSF-TDDFT with cc-pVTZ basis set. The values in parentheses are c_{HF} for each functional.

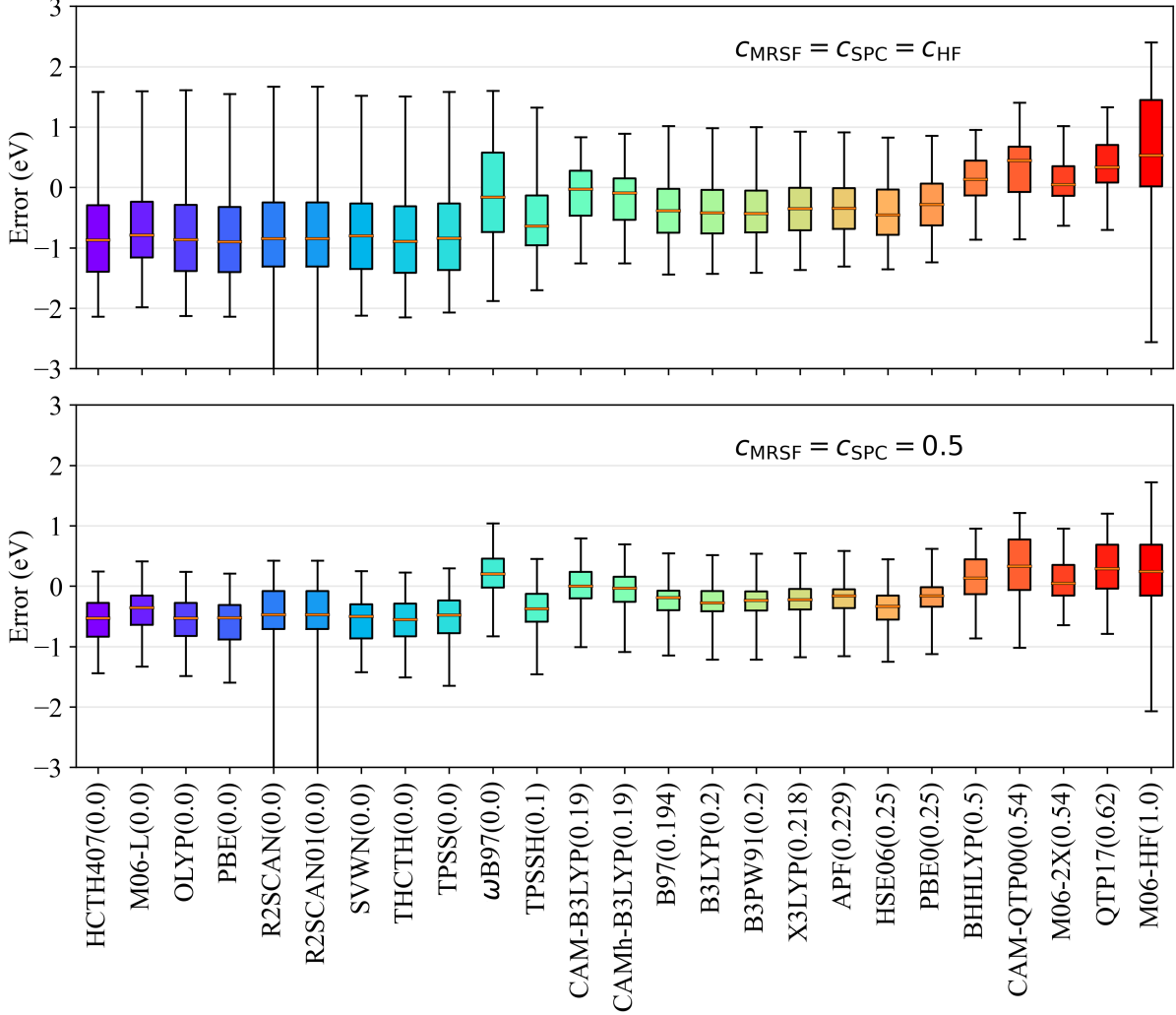


FIG. S2: The boxplot (medians, interquartile ranges, as well as whiskers) of S_1 and S_2 excited state error (in eV) relative best estimate obtained for Thiel’s molecular set as a function of XC functionals, where top figure represents the boxplot results with $c_{\text{MRSF}}=c_{\text{SPC}}=c_{\text{HF}}$, while the boxplots of bottom figure were generated with $c_{\text{MRSF}}=c_{\text{SPC}}=0.5$. All calculations were done by MRSF-TDDFT with cc-pVTZ basis set. The values in parentheses are c_{HF} for each functional. The values in parentheses are c_{HF} for each functional.

II. ORBITAL STATIONARY CONDITIONS: $\mathbf{Z}^{(k)}$ -VECTOR EQUATIONS

Two independent sets of orbital stationary conditions for singlet ($k = S$) and triplet response states ($k = T$) are defined, respectively, as

$$\sum_{\mu} \frac{\partial L^{(k)}}{\partial c_{\mu t \alpha}} c_{\mu u \alpha} + \sum_{\mu} \frac{\partial L^{(k)}}{\partial c_{\mu t \beta}} c_{\mu u \beta} = 0. \quad (1)$$

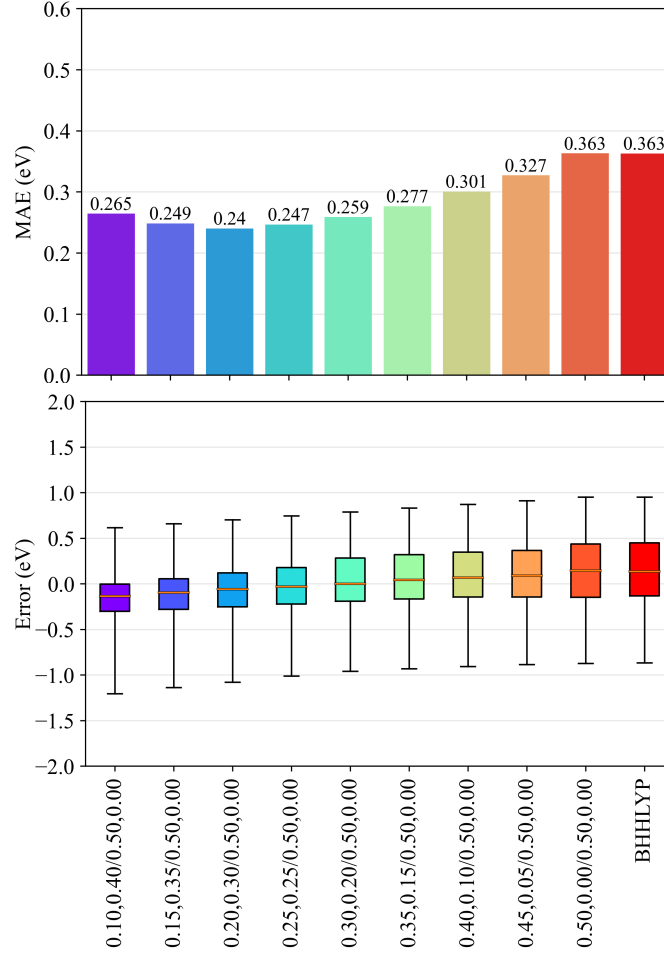


FIG. S3: The upper panel with mean absolute errors (MAE) and the bottom panel with the boxplot (medians, interquartile ranges, as well as whiskers) (in eV) of S_1 and S_2 excited states against (based on symmetry label of states) the best estimates for Thiel's molecular set as a function of range-separated exact exchange (α_1 , β_1) for SCF part at fixed ($\alpha_2=0.5$, $\beta_2=0.0$) for response part with range-separation parameter $\mu = 0.33$. All calculations were done by MRSF-TDDFT with cc-pVTZ basis set.

From this condition, the following $\mathbf{Z}^{(k)}$ -vector equation can be derived as

$$\sum_r \sum_s^{C,O} \bar{J}_{pq,rs} \bar{Z}_{rs}^{(k)} = -\bar{R}_{pq}^{(k)}, \quad p \in C, O \quad q \in O, V, \quad (2)$$

where the unique spin-independent $\mathbf{Z}^{(k)}$ vector (with the bar symbol) is introduced as:

$$\bar{Z}_{ix}^{(k)} = Z_{ix\beta'}^{(k)} \quad (3a)$$

$$\bar{Z}_{xa}^{(k)} = Z_{xa\alpha'}^{(k)} \quad (3b)$$

$$\bar{Z}_{ia}^{(k)} = Z_{ia\alpha}^{(k)} = Z_{ia\beta'}^{(k)} \quad \text{otherwise, } 0. \quad (3c)$$

The orbital Hessian $\bar{J}_{pq,rs}$ of MRSF-TDDFT takes the identical forms of SF-TDDFT^{S1} as:

$$\begin{aligned} \bar{J}_{ix,jy} &= (ix | jy) - \frac{\mathbf{c}_{\text{HF}}}{2} [(iy | jx) + (ij | xy)] + f_{ix\beta,jy\beta}^{xc} \\ &\quad - \frac{1}{2} F_{ij\beta} \delta_{xy} + \frac{1}{2} F_{xy\beta} \delta_{ij}, \end{aligned} \quad (4a)$$

$$\begin{aligned} \bar{J}_{ia,jy} &= 2 (ia | jy) - \frac{\mathbf{c}_{\text{HF}}}{2} [(iy | ja) + (ij | ya)] + f_{ia\alpha,jy\beta}^{xc} \\ &\quad + f_{ia\beta,jy\beta}^{xc} + \frac{1}{2} F_{ya\beta} \delta_{ij}, \end{aligned} \quad (4b)$$

$$\bar{J}_{xa,jy} = (xa | jy) + f_{xa\alpha,jy\beta}^{xc} - \frac{1}{2} F_{ja\alpha} \delta_{xy}, \quad (4c)$$

$$\begin{aligned} \bar{J}_{ia,jb} &= 4 (ia | jb) - \mathbf{c}_{\text{HF}} [(ib | ja) + (ij | ab)] \\ &\quad + f_{ia\alpha,jb\alpha}^{xc} + f_{ia\alpha,jb\beta}^{xc} + f_{ia\beta,jb\alpha}^{xc} + f_{ia\beta,jb\beta}^{xc} \\ &\quad + (\epsilon_a - \epsilon_i) \delta_{ij} \delta_{ab}, \end{aligned} \quad (4d)$$

$$\begin{aligned} \bar{J}_{xa,jb} &= 2 (xa | jb) - \mathbf{c}_{\text{HF}} [(xb | ja) + (jx | ab)] + f_{xa\alpha,jb\alpha}^{xc} \\ &\quad + f_{xa\alpha,jb\beta}^{xc} - \frac{1}{2} F_{jx\alpha} \delta_{ab}, \end{aligned} \quad (4e)$$

$$\begin{aligned} \bar{J}_{xa,yb} &= (xa | yb) - \frac{1}{2} [(xb | ya) + (xy | ab)] + f_{xa\alpha,yb\alpha}^{xc} \\ &\quad - \frac{1}{2} F_{xy\alpha} \delta_{ab} + \frac{1}{2} F_{ab\alpha} \delta_{xy}, \end{aligned} \quad (4f)$$

where $f_{pq\sigma,r\sigma\tau}^{xc}$ represents the matrix elements of the second functional derivatives of the exchange-correlation functional with respect to the electron density. The spin-state-specific $\bar{R}_{pq}^{(k)}$ on the right-hand side of Eq. (2) for the singlet ($k = S$) and triplet states ($k = T$) are given by:

$$\begin{aligned} \bar{R}_{ix}^{(k)} &= \frac{1}{2} H_{ix\beta}^+ [\mathbf{T}^{(k)}] + H_{ix\alpha} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] \\ &\quad - H_{xi\alpha} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] - H_{xi\beta} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}], \\ \bar{R}_{xa}^{(k)} &= \frac{1}{2} H_{xa\alpha}^+ [\mathbf{T}^{(k)}] + H_{xa\alpha} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] \\ &\quad + H_{xa\beta} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] - H_{ax\beta} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}], \\ \bar{R}_{ia}^{(k)} &= \frac{1}{2} (H_{ia\alpha}^+ [\mathbf{T}^{(k)}] + H_{ia\beta}^+ [\mathbf{T}^{(k)}]) \\ &\quad + H_{ia\alpha} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] - H_{ai\beta} [\mathbf{X}^{(k)}, \mathbf{X}^{(k)}], \end{aligned} \quad (5)$$

where

$$\begin{aligned} H_{pq\sigma}^+ [\mathbf{V}] &\equiv \sum_{rst} \{ 2 (pq | rs) + 2 f_{pq\sigma,r\sigma\tau}^{xc} \\ &\quad - \mathbf{c}_{\text{MRSF}} \delta_{\sigma\tau} [(ps | rq) + (pr | sq)] \} V_{rst}, \end{aligned} \quad (6)$$

with

$$\begin{aligned}
T_{pr\alpha}^{(k)} &\equiv - \sum_q^{O,V} U_{pq}^{(k)} X_{pq}^{(k)} U_{rq}^{(k)} X_{rq}^{(k)}, \quad p, r \in C, O, \\
T_{qs\beta}^{(k)} &\equiv \sum_p^{C,O} U_{pq}^{(k)} X_{pq}^{(k)} U_{ps}^{(k)} X_{ps}^{(k)}, \quad q, s \in O, V.
\end{aligned} \tag{7}$$

And the $H_{tu\sigma}[\mathbf{X}^{(k)}, \mathbf{X}^{(k)}]$ of Eq. (5) is defined as

$$\begin{aligned}
H_{tu\sigma}[\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] &\equiv H_{tu\sigma}^{(0)}[\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] \\
&+ \sum_{xy} H_{tu\sigma}^{\text{intra}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{Cy}^{(k)}] + \sum_{xy} H_{tu\sigma}^{\text{intra}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{yV}^{(k)}] \\
&+ \sum_x H_{tu\sigma}^{\text{inter}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{xV}^{(k)}] + \sum_x H_{tu\sigma}^{\text{inter}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{Cx}^{(k)}],
\end{aligned} \tag{8}$$

where

$$\begin{aligned}
H_{tu\alpha}^{(0)}[\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] &\equiv \sum_r^{C,O} \sum_{qs}^{O,V} U_{tq}^{(k)} X_{tq}^{(k)} \{ \delta_{ur} F_{qs\beta} - \delta_{qs} F_{ura} \\
&\quad - \mathbf{c}_{\text{MRSE}}(ur | sq) \} U_{rs}^{(k)} X_{rs}^{(k)}, \\
H_{tu\beta}^{(0)}[\mathbf{X}^{(k)}, \mathbf{X}^{(k)}] &\equiv \sum_{pr}^{C,O} \sum_s^{O,V} U_{pt}^{(k)} X_{pt}^{(k)} \{ \delta_{pr} F_{us\beta} - \delta_{us} F_{pra} \\
&\quad - \mathbf{c}_{\text{MRSE}}(pr | su) \} U_{rs}^{(k)} X_{rs}^{(k)},
\end{aligned} \tag{9}$$

and

$$\begin{aligned}
H_{tu\alpha}^{\text{intra}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{Cy}^{(k)}] &\equiv (-1)^{1-\delta_{xy}} \sum_r^C \sum_{qs}^O U_{tq}^{Cx} X_{tq}^{(k)} H_{uq,rs}^{(k)\text{intra}} \\
&\quad \times U_{rs}^{Cy} X_{rs}^{(k)}, \\
H_{tu\alpha}^{\text{intra}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{yV}^{(k)}] &\equiv (-1)^{1-\delta_{xy}} \sum_r^O \sum_{qs}^V U_{tq}^{xV} X_{tq}^{(k)} H_{uq,rs}^{(k)\text{intra}} \\
&\quad \times U_{rs}^{yV} X_{rs}^{(k)}, \\
H_{tu\alpha}^{\text{inter}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{yV}^{(k)}] &\equiv \sum_{rq}^O \sum_s^V U_{tq}^{Cx} X_{tq}^{(k)} H_{uq,rs}^{(k)\text{inter}} U_{rs}^{yV} X_{rs}^{(k)}, \\
H_{tu\alpha}^{\text{inter}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{Cy}^{(k)}] &\equiv \sum_r^C \sum_s^O \sum_q^V U_{tq}^{xV} X_{tq}^{(k)} H_{uq,rs}^{(k)\text{inter}} U_{rs}^{Cy} X_{rs}^{(k)}, \\
H_{tu\beta}^{\text{intra}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{Cy}^{(k)}] &\equiv (-1)^{1-\delta_{xy}} \sum_{pr}^C \sum_s^O U_{pt}^{Cx} X_{pt}^{(k)} H_{pu,rs}^{(k)\text{intra}}
\end{aligned} \tag{10}$$

$$\begin{aligned}
& \times U_{rs}^{Cy} X_{rs}^{(k)}, \\
H_{tu\beta}^{\text{intra}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{yV}^{(k)}] & \equiv (-1)^{1-\delta_{xy}} \sum_{pr}^O \sum_s^V U_{pt}^{xV} X_{pt}^{(k)} H_{pu,rs}^{(k)\text{intra}} \\
& \times U_{rs}^{yV} X_{rs}^{(k)}, \\
H_{tu\beta}^{\text{inter}}[\mathbf{X}_{Cx}^{(k)}, \mathbf{X}_{yV}^{(k)}] & \equiv \sum_p^C \sum_r^O \sum_s^V U_{pt}^{Cx} X_{pt}^{(k)} H_{pu,rs}^{(k)\text{inter}} U_{rs}^{yV} X_{rs}^{(k)}, \\
H_{tu\beta}^{\text{inter}}[\mathbf{X}_{xV}^{(k)}, \mathbf{X}_{Cy}^{(k)}] & \equiv \sum_r^O \sum_{pr} U_{pt}^{xV} X_{pt}^{(k)} H_{pu,rs}^{(k)\text{inter}} U_{rs}^{Cy} X_{rs}^{(k)}. \tag{11}
\end{aligned}$$

Four terms on the right-hand side of Eq. (III.12) except for the first term are derived from the spin-pairing coupling in Eq. (II.15). Without these terms, all equations for the $\mathbf{Z}^{(k)}$ -vector equation are almost same as those of SF-TDDFT.^{S1} Only the difference is using the expanded excitation amplitudes, $U_{pq}^{(k)} X_{pq}^{(k)}$, in MRSF-TDDFT. This is a great advantage since one can simply utilize the same existing routines for SF-TDDFT.

III. GRADIENT OF MRSF-TDDFT

From the stationary condition of Lagrangian for a nuclear coordinate (ξ) of

$$\frac{\partial L^{(k)}}{\partial \xi} = 0, \tag{12}$$

the analytic gradient of the excitation energy ($\Omega_{(k)}^{\xi}$) can be obtained by:

$$\begin{aligned}
\Omega_{(k)}^{\xi} & = \sum_{\mu\nu\sigma} h_{\mu\nu}^{\xi} P_{\mu\nu\sigma}^{(k)} - \sum_{\mu\nu\sigma} S_{\mu\nu}^{\xi} W_{\mu\nu\sigma}^{(k)} \\
& + \sum_{\mu\nu\sigma, \kappa\lambda\tau} (\mu\nu | \kappa\lambda)^{\xi} \Gamma_{\mu\nu\sigma, \kappa\lambda\tau}^{(k)}, \tag{13}
\end{aligned}$$

where the superscript ξ denotes the derivative with respect to the nuclear coordinate. $h_{\mu\nu}^{\xi}$ and $(\mu\nu | \kappa\lambda)^{\xi}$ are the derivatives of one- and two-electron integrals in AO basis. $S_{\mu\nu}^{\xi}$ is the derivative of AO overlap integral. $P_{\mu\nu\sigma}^{(k)}$ and $W_{\mu\nu\sigma}^{(k)}$ are

$$P_{\mu\nu\alpha}^{(k)} \equiv \sum_{pq}^{C,O} c_{\mu p\alpha} P_{pq\alpha}^{(k)} c_{\nu q\alpha}, \tag{14a}$$

$$P_{\mu\nu\beta}^{(k)} \equiv \sum_{pq}^{O,V} c_{\mu p\beta} P_{pq\beta}^{(k)} c_{\nu q\beta}, \tag{14b}$$

$$W_{\mu\nu\alpha}^{(k)} \equiv \sum_{p \leq q} c_{\mu p\alpha} W_{pq\alpha}^{(k)} c_{\nu q\alpha}, \tag{15a}$$

$$W_{\mu\nu\beta}^{(k)} \equiv \sum_{p \leq q} c_{\mu p \beta} W_{pq\beta}^{(k)} c_{\nu q \beta}. \quad (15b)$$

In addition, $\Gamma_{\mu\nu\sigma,\kappa\lambda\tau}^{(k)}$ are given by

$$\begin{aligned} & \Gamma_{\mu\nu\sigma,\kappa\lambda\tau}^{(k)} \\ &= \frac{1}{2} [2P_{\mu\nu\sigma}^{(k)} D_{\kappa\lambda\tau} - \mathbf{c}_{\text{HF}} \delta_{\sigma\tau} (P_{\mu\kappa\sigma}^{(k)} D_{\nu\lambda\sigma} + P_{\mu\lambda\sigma}^{(k)} D_{\nu\kappa\sigma}) \\ & \quad - \mathbf{c}_{\text{MRSF}} \delta_{\sigma\alpha} \delta_{\tau\beta} (X_{\mu\lambda}^{(k)} X_{\nu\kappa}^{(k)} + X_{\mu\kappa}^{(k)} X_{\nu\lambda}^{(k)})] \\ &+ \text{sgn}(k) \mathbf{c}_{\text{SPC}} \delta_{\sigma\alpha} \delta_{\tau\beta} \times \\ & \quad [\{ (\mathbf{X}_{O1V}^{\text{intra}})^{(k)}_{\mu\lambda} - (\mathbf{X}_{O2V}^{\text{intra}})^{(k)}_{\mu\lambda} \} \{ (\mathbf{X}_{O1V}^{\text{intra}})^{(k)}_{\kappa\nu} - (\mathbf{X}_{O2V}^{\text{intra}})^{(k)}_{\kappa\nu} \} \\ & \quad + \{ (\mathbf{X}_{CO1}^{\text{intra}})^{(k)}_{\mu\lambda} - (\mathbf{X}_{CO2}^{\text{intra}})^{(k)}_{\mu\lambda} \} \{ (\mathbf{X}_{CO1}^{\text{intra}})^{(k)}_{\kappa\nu} - (\mathbf{X}_{CO2}^{\text{intra}})^{(k)}_{\kappa\nu} \} \\ & \quad + (\mathbf{X}_{CO1}^{\text{inter}})^{(k)}_{\mu\nu} (\mathbf{X}_{O2V}^{\text{inter}})^{(k)}_{\kappa\lambda} + (\mathbf{X}_{CO2}^{\text{inter}})^{(k)}_{\mu\nu} (\mathbf{X}_{O1V}^{\text{inter}})^{(k)}_{\kappa\lambda} \\ & \quad + (\mathbf{X}_{O2V}^{\text{inter}})^{(k)}_{\mu\nu} (\mathbf{X}_{CO1}^{\text{inter}})^{(k)}_{\kappa\lambda} + (\mathbf{X}_{O1V}^{\text{inter}})^{(k)}_{\mu\nu} (\mathbf{X}_{CO2}^{\text{inter}})^{(k)}_{\kappa\lambda} \\ & \quad - (\mathbf{X}_{CO1}^{\text{inter}})^{(k)}_{\mu\lambda} (\mathbf{X}_{O2V}^{\text{inter}})^{(k)}_{\nu\kappa} - (\mathbf{X}_{CO2}^{\text{inter}})^{(k)}_{\mu\lambda} (\mathbf{X}_{O1V}^{\text{inter}})^{(k)}_{\nu\kappa} \\ & \quad - (\mathbf{X}_{O2V}^{\text{inter}})^{(k)}_{\mu\lambda} (\mathbf{X}_{CO1}^{\text{inter}})^{(k)}_{\nu\kappa} - (\mathbf{X}_{O1V}^{\text{inter}})^{(k)}_{\mu\lambda} (\mathbf{X}_{CO2}^{\text{inter}})^{(k)}_{\nu\kappa}], \end{aligned} \quad (16)$$

where

$$D_{\mu\nu\alpha} \equiv \sum_p^{C,O} c_{\mu p \alpha} c_{\nu p \alpha}, \quad (17a)$$

$$D_{\mu\nu\beta} \equiv \sum_p^C c_{\mu p \beta} c_{\nu p \beta}, \quad (17b)$$

$$X_{\mu\nu}^{(k)} \equiv \sum_p^{C,O,O,V} \sum_q c_{\mu p \alpha} U_{pq}^{(k)} X_{pq}^{(k)} c_{\nu q \beta}, \quad (18)$$

and

$$\begin{aligned} (\mathbf{X}_{OmV}^{\text{intra}})^{(k)}_{\mu\nu} &\equiv \sum_p^O \sum_q^V c_{\mu p \alpha} U_{pq}^{OmV} X_{pq}^{(k)} c_{\nu q \beta}, \\ (\mathbf{X}_{COm}^{\text{intra}})^{(k)}_{\mu\nu} &\equiv \sum_p^C \sum_q^O c_{\mu p \alpha} U_{pq}^{COm} X_{pq}^{(k)} c_{\nu q \beta}, \\ (\mathbf{X}_{OmV}^{\text{inter}})^{(k)}_{\mu\nu} &\equiv \sum_p^O \sum_q^V c_{\mu p \alpha} U_{pq}^{OmV} X_{pq}^{(k)} c_{\nu q \beta}, \\ (\mathbf{X}_{COm}^{\text{inter}})^{(k)}_{\mu\nu} &\equiv \sum_p^C \sum_q^O c_{\mu p \alpha} U_{pq}^{COm} X_{pq}^{(k)} c_{\nu q \beta}. \end{aligned} \quad (19)$$

Finally, the gradient of the ground state energy is given by:

$$\begin{aligned}
E^{\xi} &= \sum_{\mu\nu\sigma} h_{\mu\nu}^{\xi} D_{\mu\nu\sigma} - \sum_{\mu\nu\sigma} S_{\mu\nu}^{\xi} W'_{\mu\nu\sigma} \\
&+ \sum_{\mu\nu\sigma,\kappa\lambda\tau} (\mu\nu|\kappa\lambda)^{\xi} \Gamma'_{\mu\nu\sigma,\kappa\lambda\tau},
\end{aligned} \tag{20}$$

where

$$\Gamma'_{\mu\nu\sigma,\kappa\lambda\tau} = \frac{1}{2} (D_{\mu\nu\sigma} D_{\kappa\lambda\tau} - c_{\text{HF}} \delta_{\sigma\tau} D_{\mu\lambda\sigma} D_{\nu\kappa\sigma}). \tag{21}$$

$$W'_{\mu\nu\sigma} = \sum_{p,q} c_{\mu p\sigma} F_{pq\sigma} c_{\nu q\sigma} \tag{22}$$

IV. NON-ADIABATIC DYNAMICS WITH MRSF-TDDFT

The three-state NAMD simulations were initiated by sampling the Wigner function of a canonical ensemble^{S2,3} at T = 300K around the S₀ equilibrium geometry. In this study, NAMD has been performed based on the fewest-switches surface-hopping algorithm,^{S4} and nonadiabatic coupling vectors are computed numerically by using a fast overlap calculation^{S5} using the locally modified GAMESS. Velocity Verlet is used for integration. The energy conservation during the hops was ensured by rescaling the velocities. Hundred trajectories were propagated using the NVE ensemble with a time-step size of 0.5 fs until 200 fs for a propagation of the nuclear degrees of freedom and with a sub-time-step size 10⁻⁵ fs for a propagation of the electronic degrees of freedom.^{S6} No corrections for decoherence were applied.

	IP/eV
Exp	8.8 ^{S7,8}
Orbital Energies of ROHF Reference	
MRSF/BH&HLYP	6.4
MRSF/DTCAM-AEE	6.2
MRSF/DTCAM-VEE	6.2
IP by EKT-MRSF	
EKT-MRSF/BH&HLYP	7.9
EKT-MRSF/DTCAM-VEE	8.2
EKT-MRSF/DTCAM-AEE	8.7

TABLE S1: The HOMO energies from MRSF and electron binding energies (eBEs) from EKT-MRSF with BH&HLYP, DTCAM-AEE, and DTCAM-VEE functionals and 6-31G(d) basis set at the MRSF/6-31G(d)/BH&HLYP optimized S_0 equilibrium geometry of thymine. The symmetry labels correspond to the C_s symmetry group.

V. PERFORMANCE OF IONIZATION POTENTIAL AND ELECTRON AFFINITY

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