# Efficient constrained DFT implementation for condensed phase electron transfer MD simulations[1]

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Electron transfer (ET) parameters directly from two-state MD simulations with explicit solvent

Example: Intramolecular ET in QTTFQ⁻ (258 water, 12 ps total, 0.5 fs step, 384 MPI cores)

$$E_{\mathrm{CDFT}}[\rho,\xi] = \max_{\xi} \min_{\rho} \left\{ E_{\mathrm{KS}}[\rho] + \xi\left(\int w(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} - N_c\right)\right\}$$

$$IS \rightleftharpoons FS + e^-$$

$$|H_{ab}| \approx |\langle \Phi_{\mathrm{IS}} | \mathcal{H}_{\mathrm{CDFT}} | \Phi_{\mathrm{FS}}\rangle|$$
$$\Delta E = E_{\mathrm{FS}} - E_{\mathrm{IS}}$$
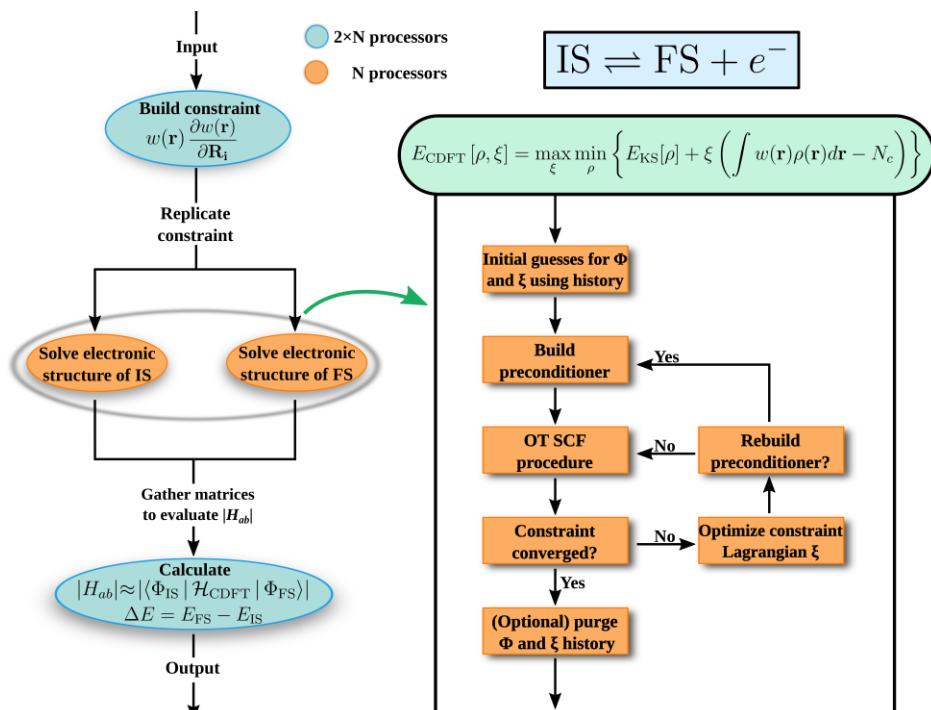
Code not yet in trunk, but available at
https://github.com/nholmber/cp2k-cdft-dev

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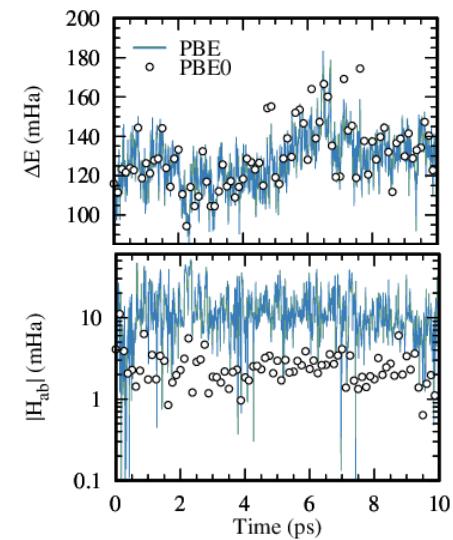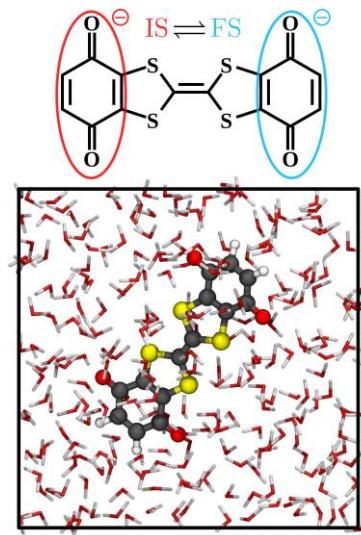
1. Holmberg, N.; Laasonen, K.; *J. Chem. Theory Comput.*, Just Accepted Manuscript, DOI: 10.1021/acs.jctc.6b01085