Importance of the reorganization energy barrier in computational design of porphyrin-based solar cells with cobalt-based redox mediators

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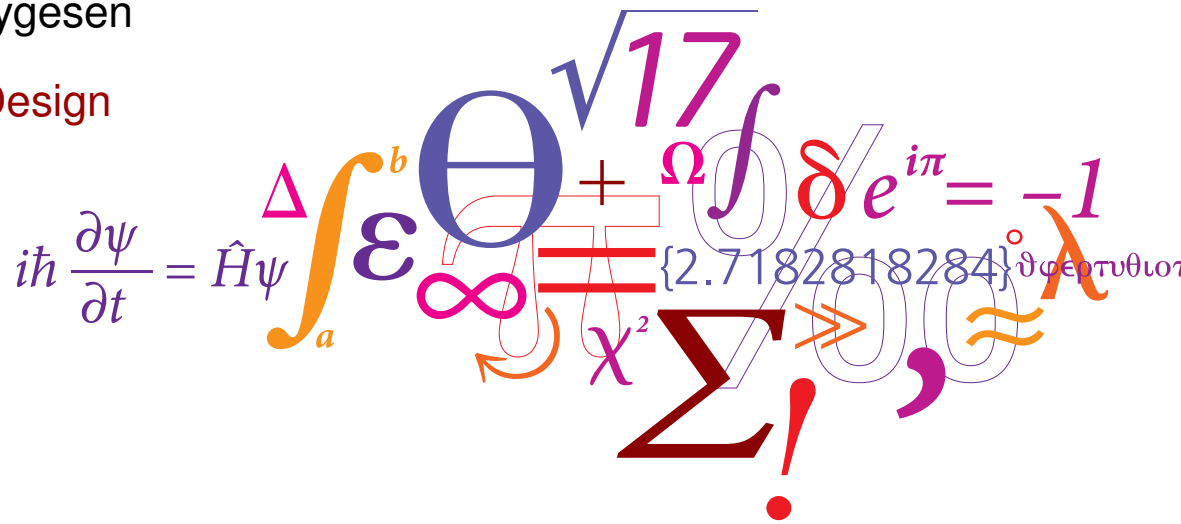

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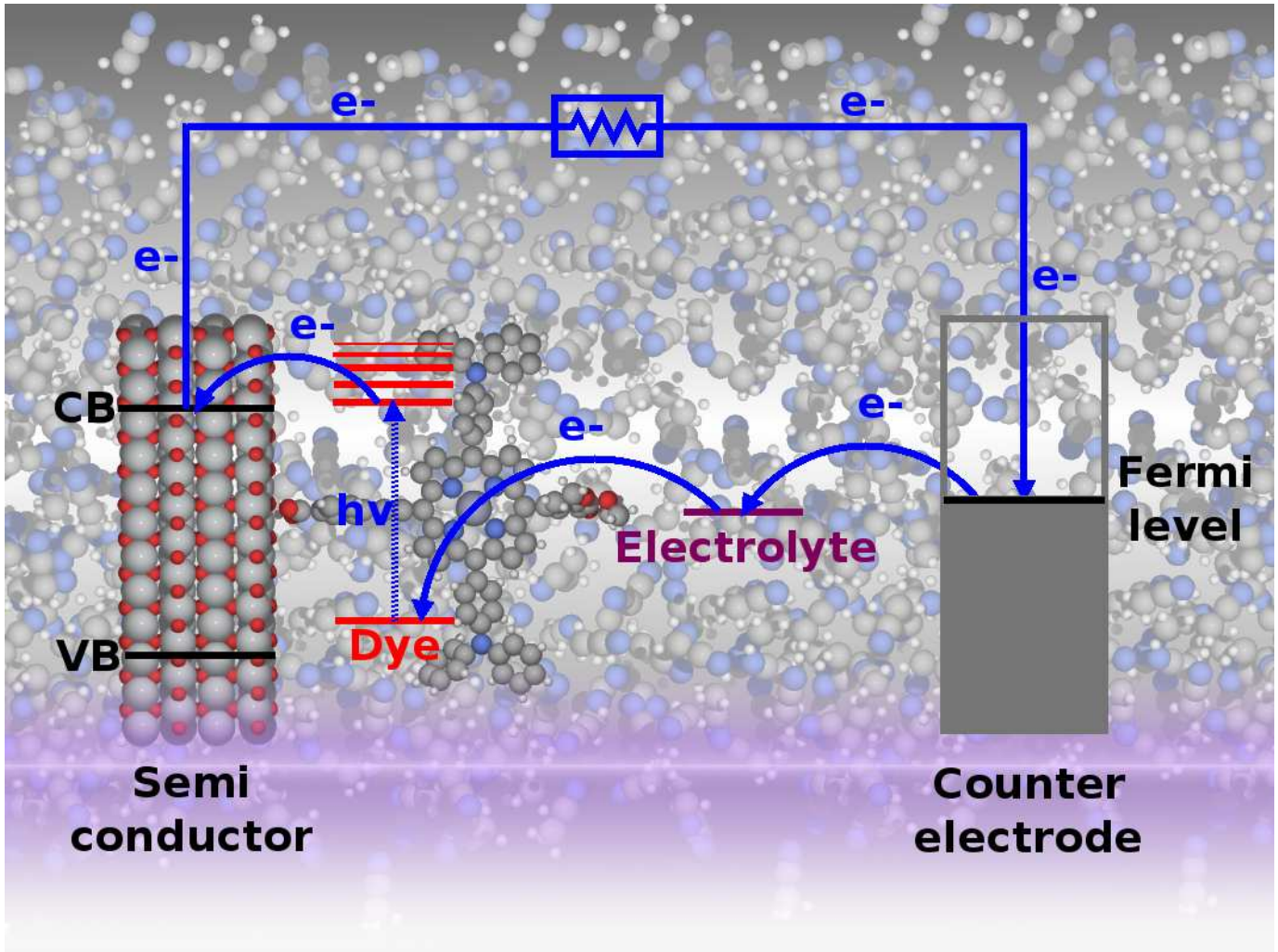
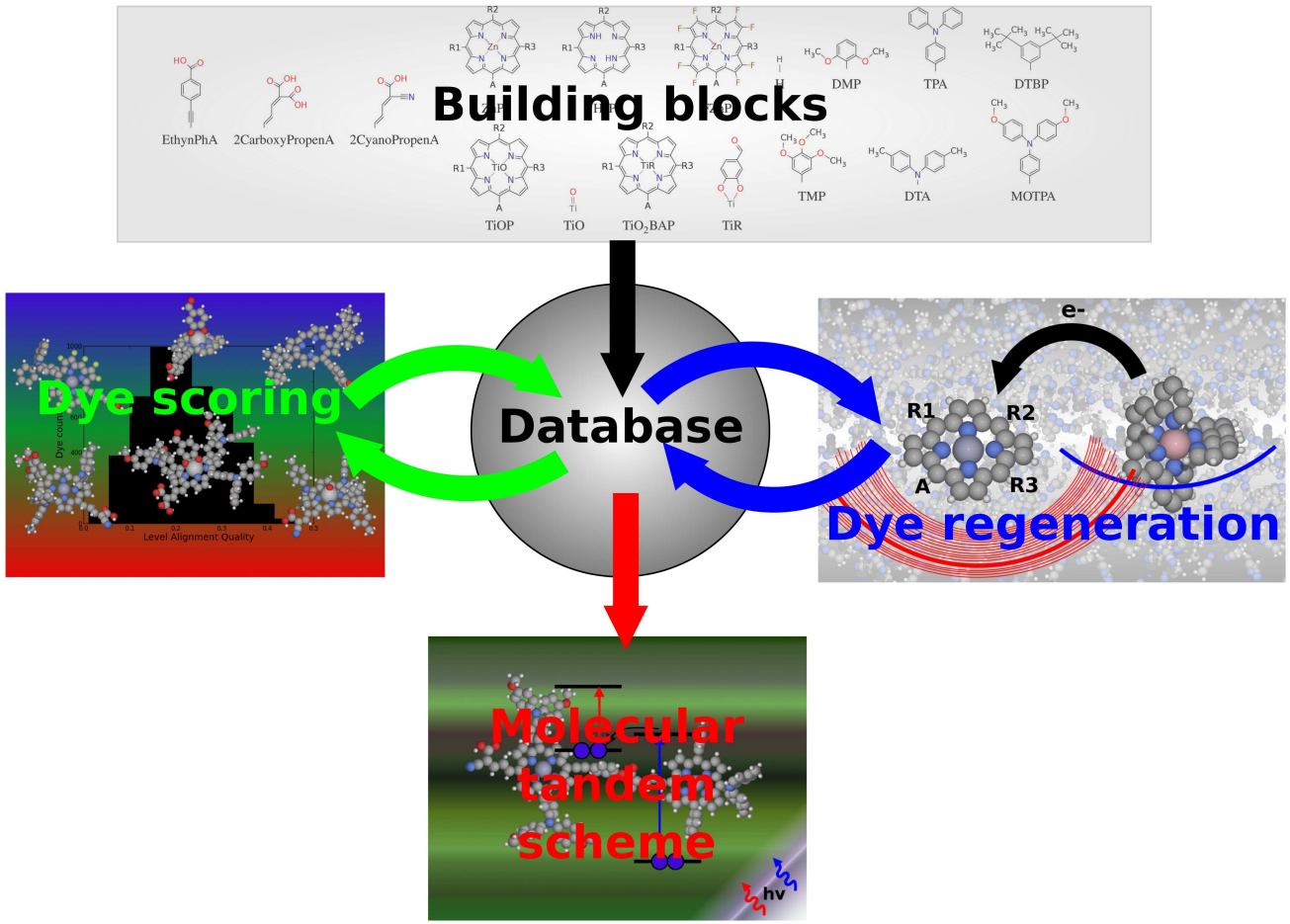
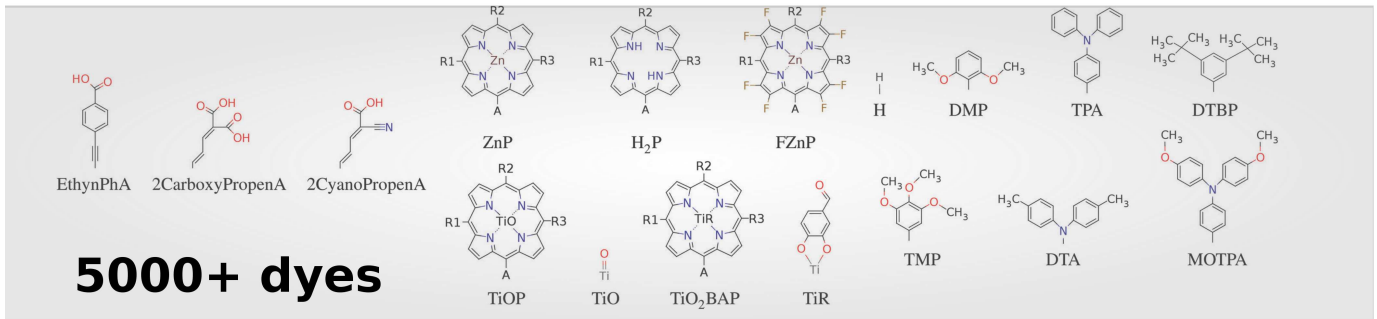
Dye Sensitized Solar Cells

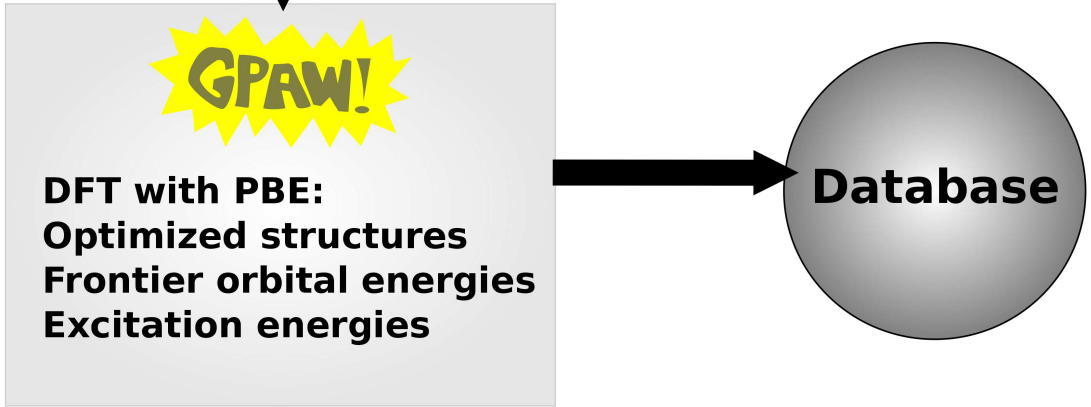


Using computational screening



Building blocks

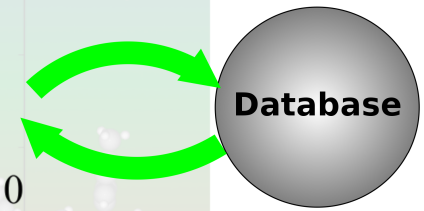




Dye scoring

$$\eta = \frac{eV_{\mathrm{oc}} \int_{E_{\mathrm{c}}-E_{\mathrm{H}}}^{\infty} \Theta(E - E_1) \cdot I_{\mathrm{solar}}(E)\mathrm{d}E}{\int_0^{\infty} E \cdot I_{\mathrm{solar}}(E)\mathrm{d}E}$$

$$\Theta(E - E_1) = \begin{cases} 1 & \text{for} \quad E - E_1 \geq 0 \\ 0 & \text{for} \quad E - E_1 < 0 \end{cases}$$



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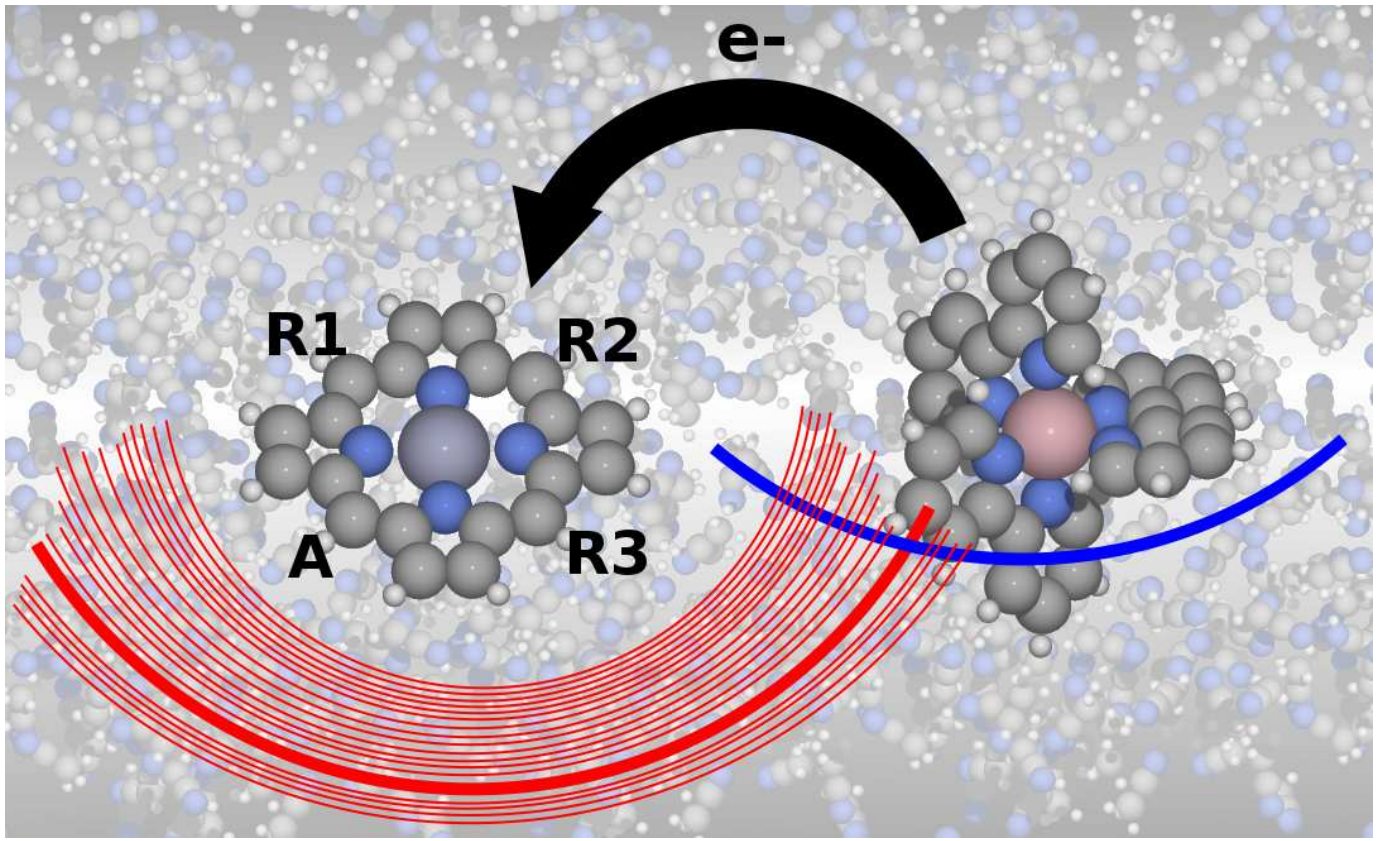
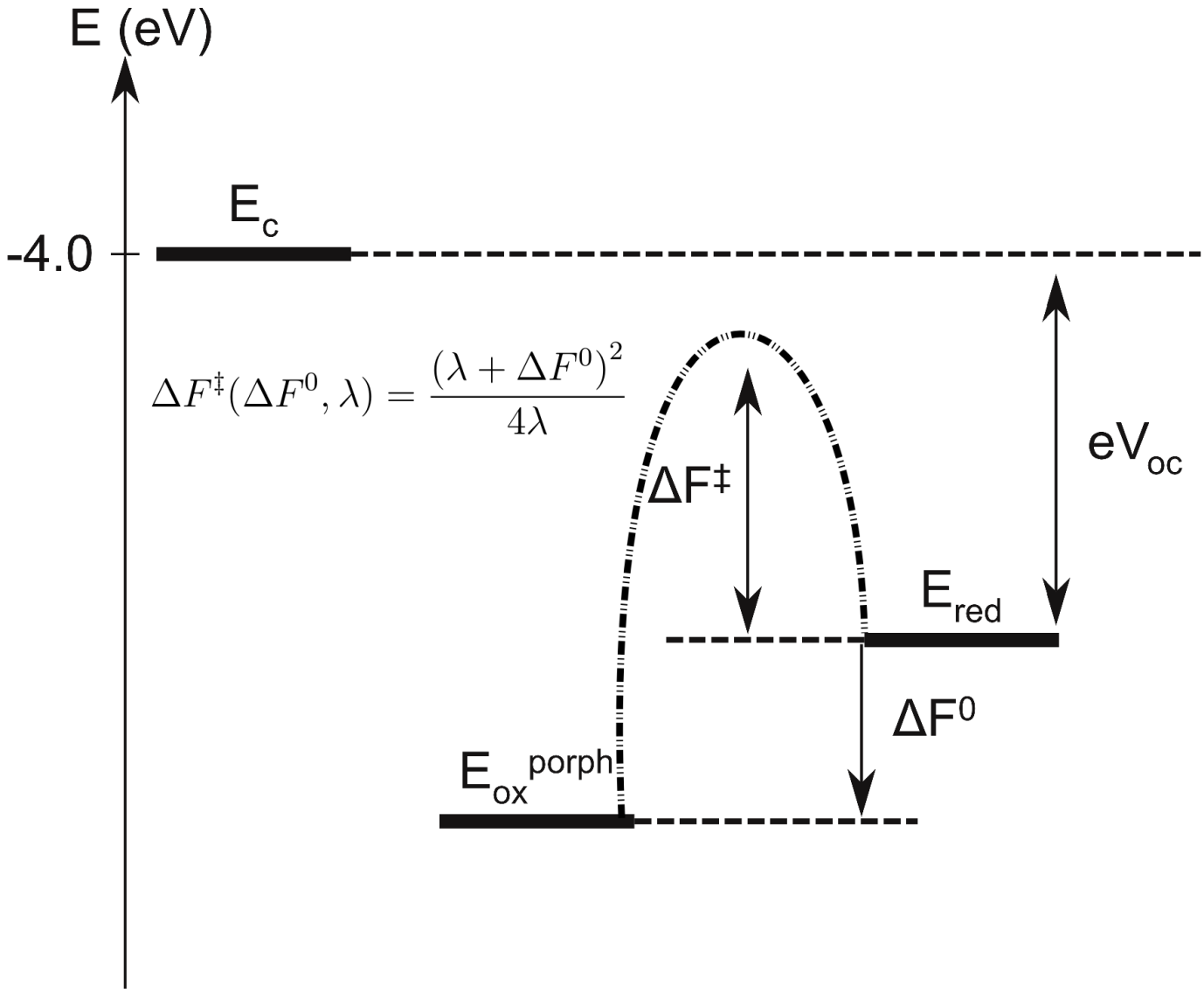
K. B. Ørnsø, C. S. Pedersen, J. M. Garcia-Lastra, and K. S. Thygesen. *Phys. Chem. Chem. Phys.*, **2014**, *16*, 16246–16254

Include regeneration electron transfer?

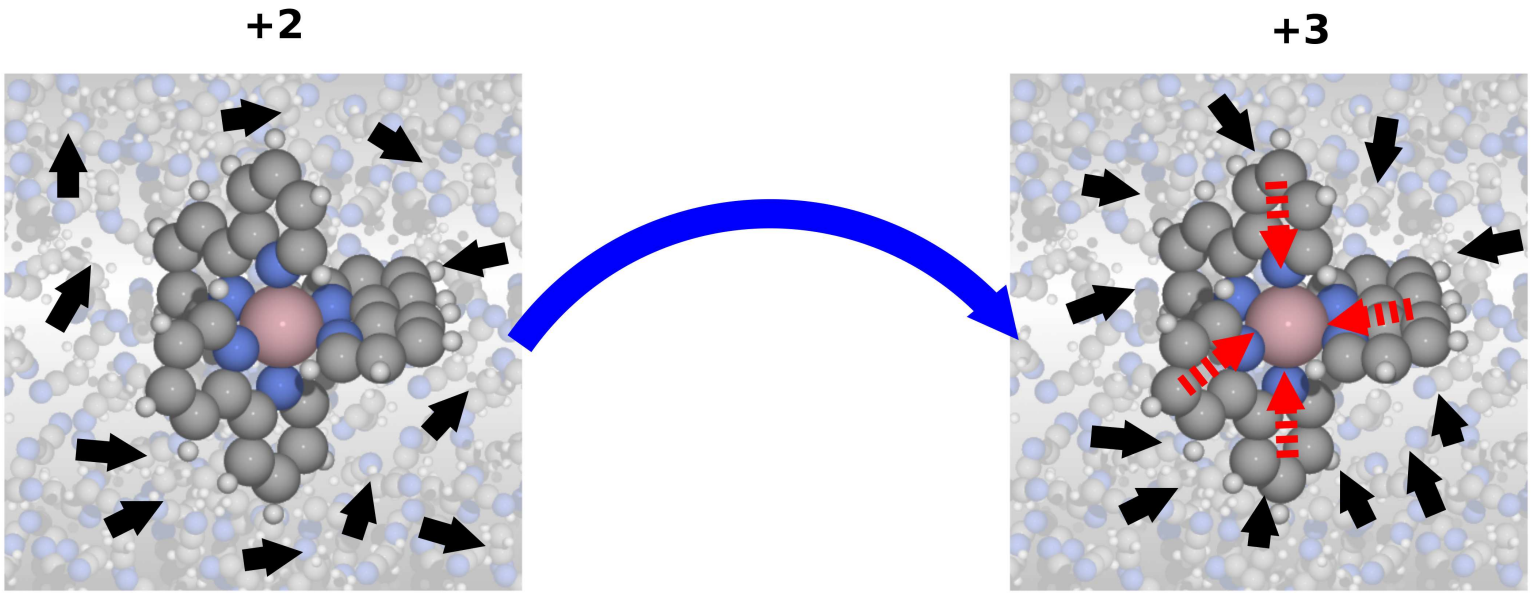


Dye regeneration

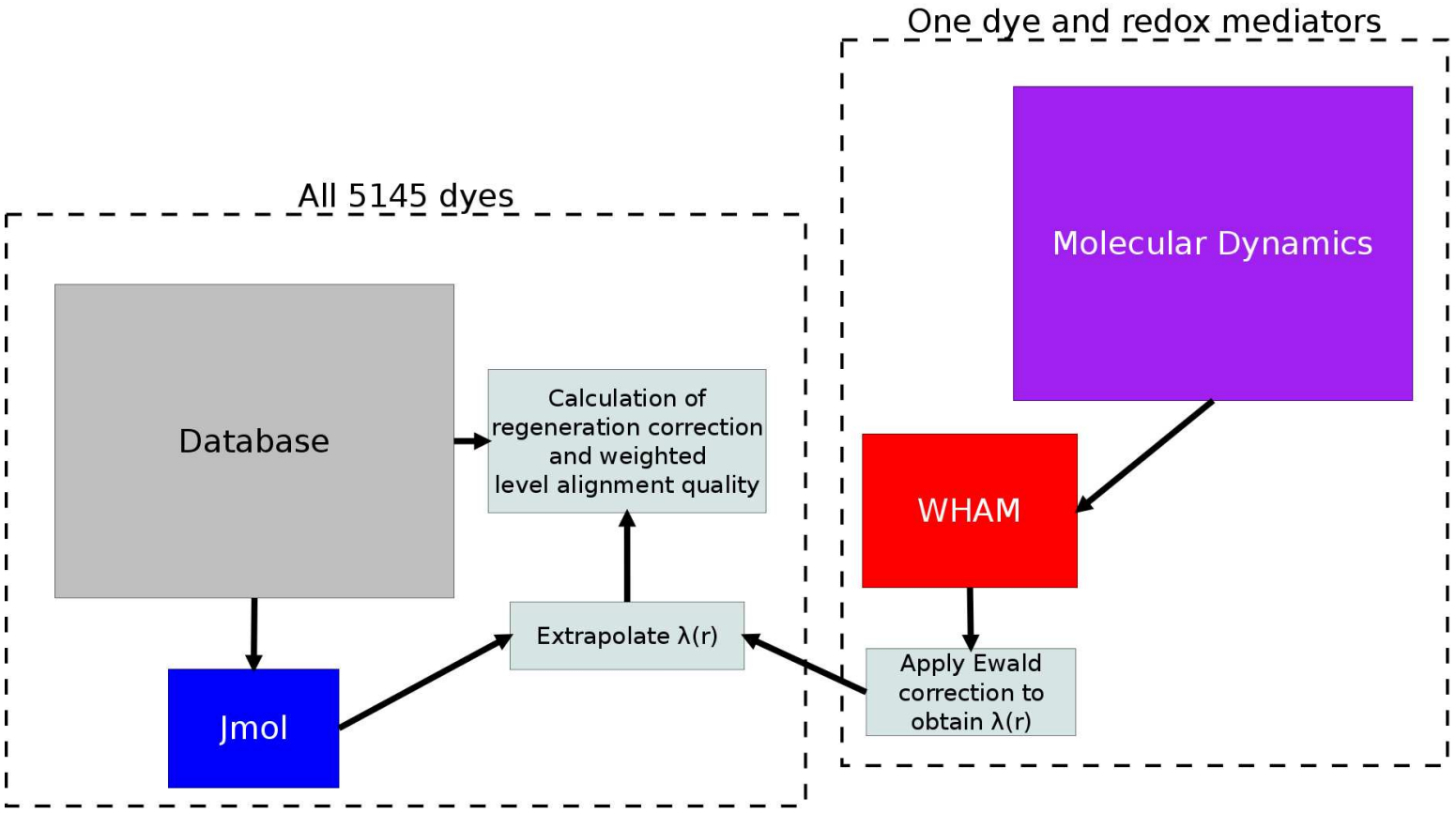


Dye regeneration

$$\lambda = \lambda^{\mathrm{in}} + \lambda^{\mathrm{out}}$$



Dye regeneration



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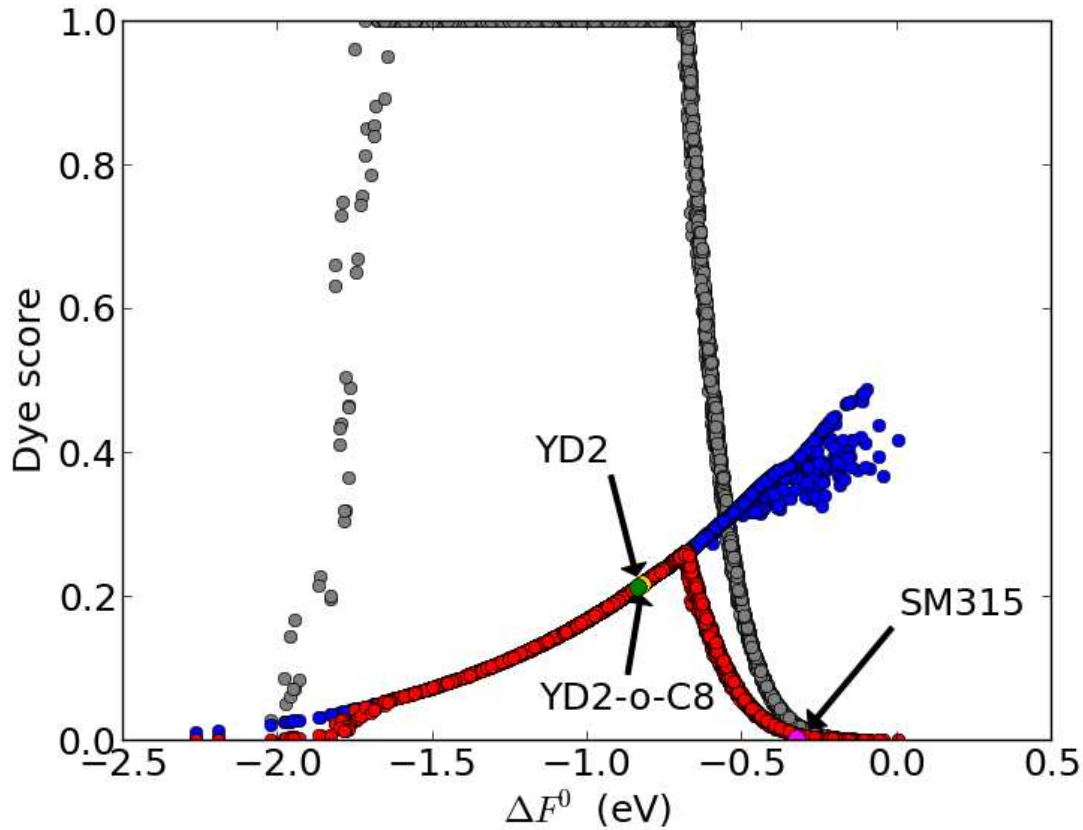
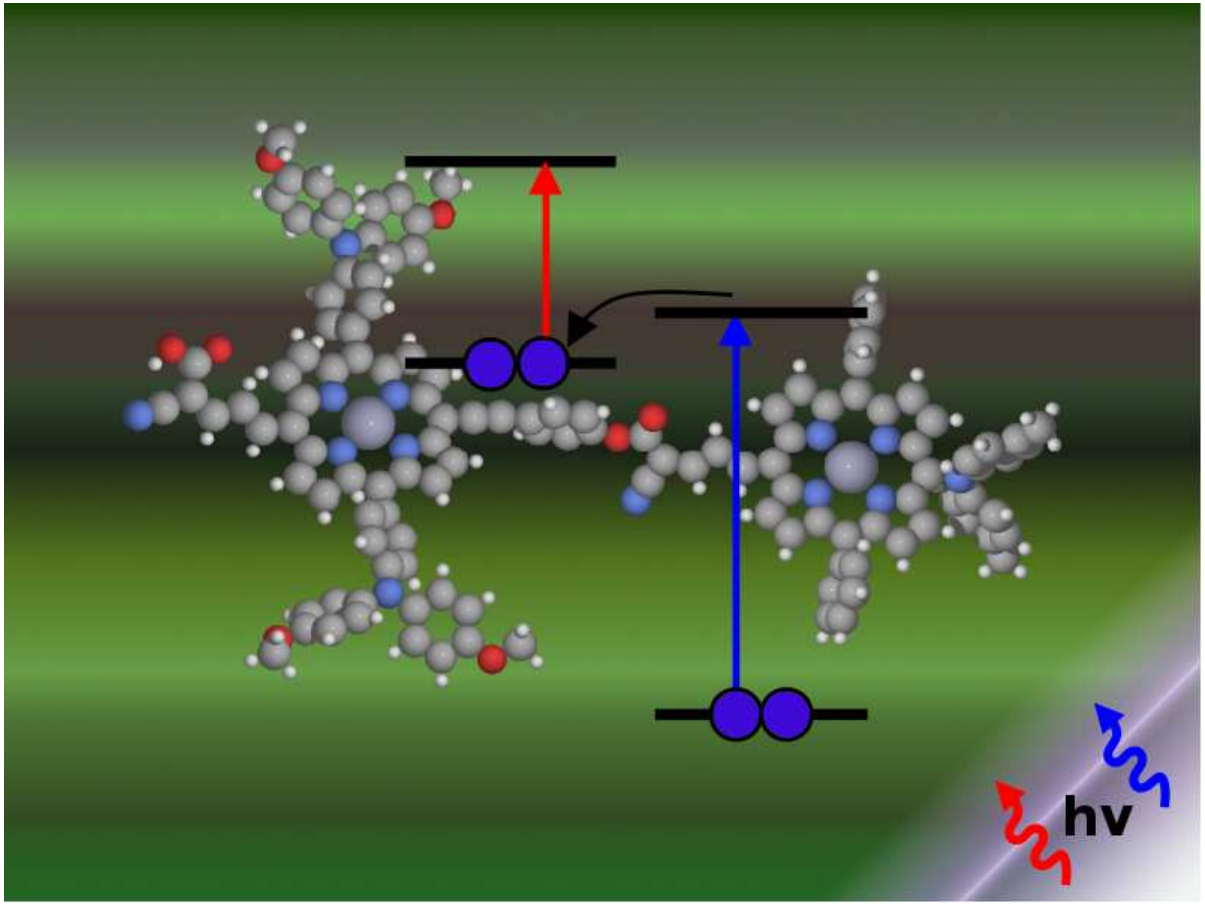
Dye regeneration

$$C' = \begin{cases} 1 & \text{for} \quad \Delta F^{\ddagger} \leq 0.05\,\text{eV} \\ \exp\left(\frac{-\Delta F^{\ddagger}(\Delta F^{0},\lambda)+0.05\,\text{eV}}{k_B T}\right) & \text{for} \quad \Delta F^{\ddagger} > 0.05\,\text{eV} \end{cases}$$



Molecular tandem scheme



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Thank you!

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Thank you for your attention!