Excitonic Configuration Interaction

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CATALIGHT

FWF

DFG

1 QM calculation on each chromophore with different embedding schemes

Multichromophoric systems

S_0 S_1 S_2 ...

2 Building the excitonic basis

Mg^{2+} in G-quadruplex

ESCF-ECIS
Full-system QM

ESCF-ECISD
Full-system QM

ESCF

ECIS

ECISD

3 Calculation of full-system Hamiltonian in excitonic basis
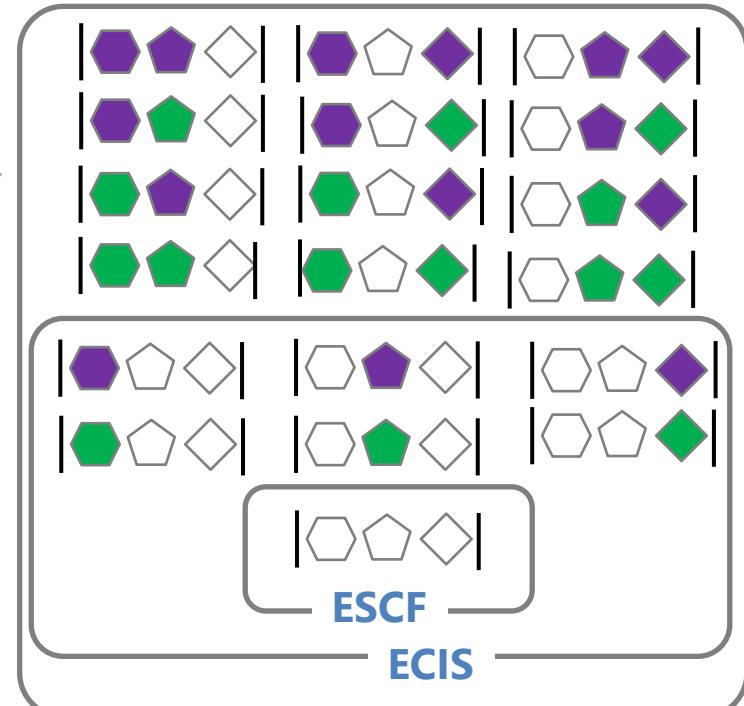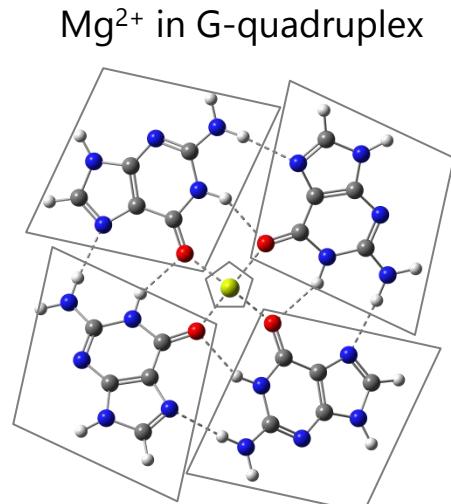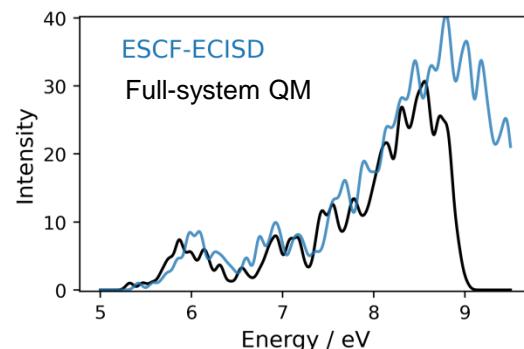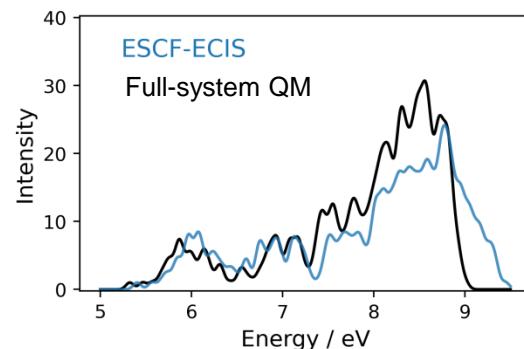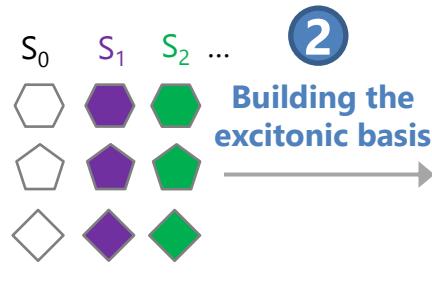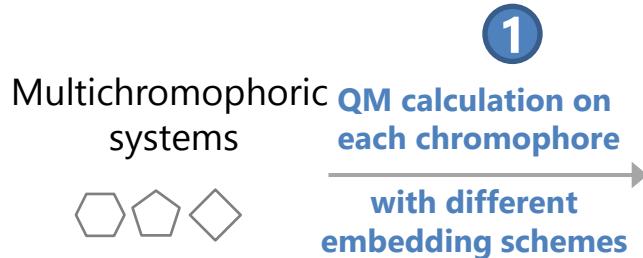
4 Diagonalization

$$\begin{pmatrix} H_{00} & \mathbf{H}_{0S} & \mathbf{H}_{0D} & \cdots \\ \mathbf{H}_{S0} & \mathbf{H}_{SS} & \mathbf{H}_{SD} & \cdots \\ \mathbf{H}_{D0} & \mathbf{H}_{DS} & \mathbf{H}_{DD} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$