Supplementary Material to the "Modeling Molecular J and H Aggregates using Multiple-Davydov D2 Ansatz"

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Absorption spectra of model J and H aggregate

In the following Figures we present absorption spectra of vibronic model J and H aggregates in an open and closed chain configuration, computed with an increasing depth, M, of the mD_2 Ansatz. Aggregate consists of 10 sites with 1 vibrational mode, of frequency $\omega = 500$ cm^{-1}, per site. Mode Huang-Rhys factor is set to $S = 1$. We vary the nearest neighbor coupling J from 0 cm^{-1} to ± 1000 cm^{-1} with step size of ± 250 cm^{-1}. Vibrational mode thermal energy $k_{\mathrm{B}}T$ is changed from 250 cm^{-1} to 1000 cm^{-1} with step of 250 cm^{-1}.

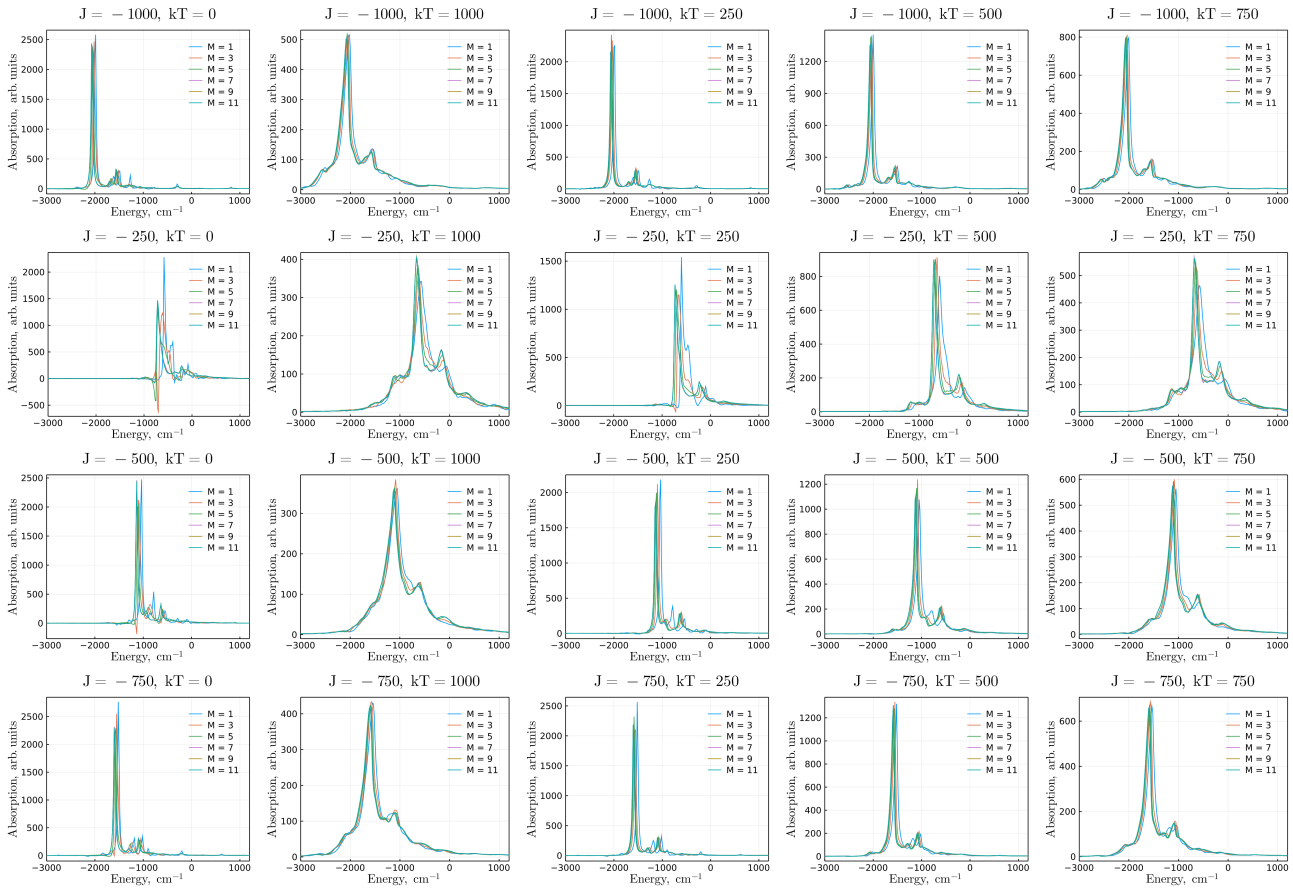

Figure 1. Absorption spectra of model J aggregate in an *open* chain configuration, computed with mD_2 Ansatz depth M, nearest neighbor coupling J and vibrational mode thermal energy $k_{\mathrm{B}}T$.

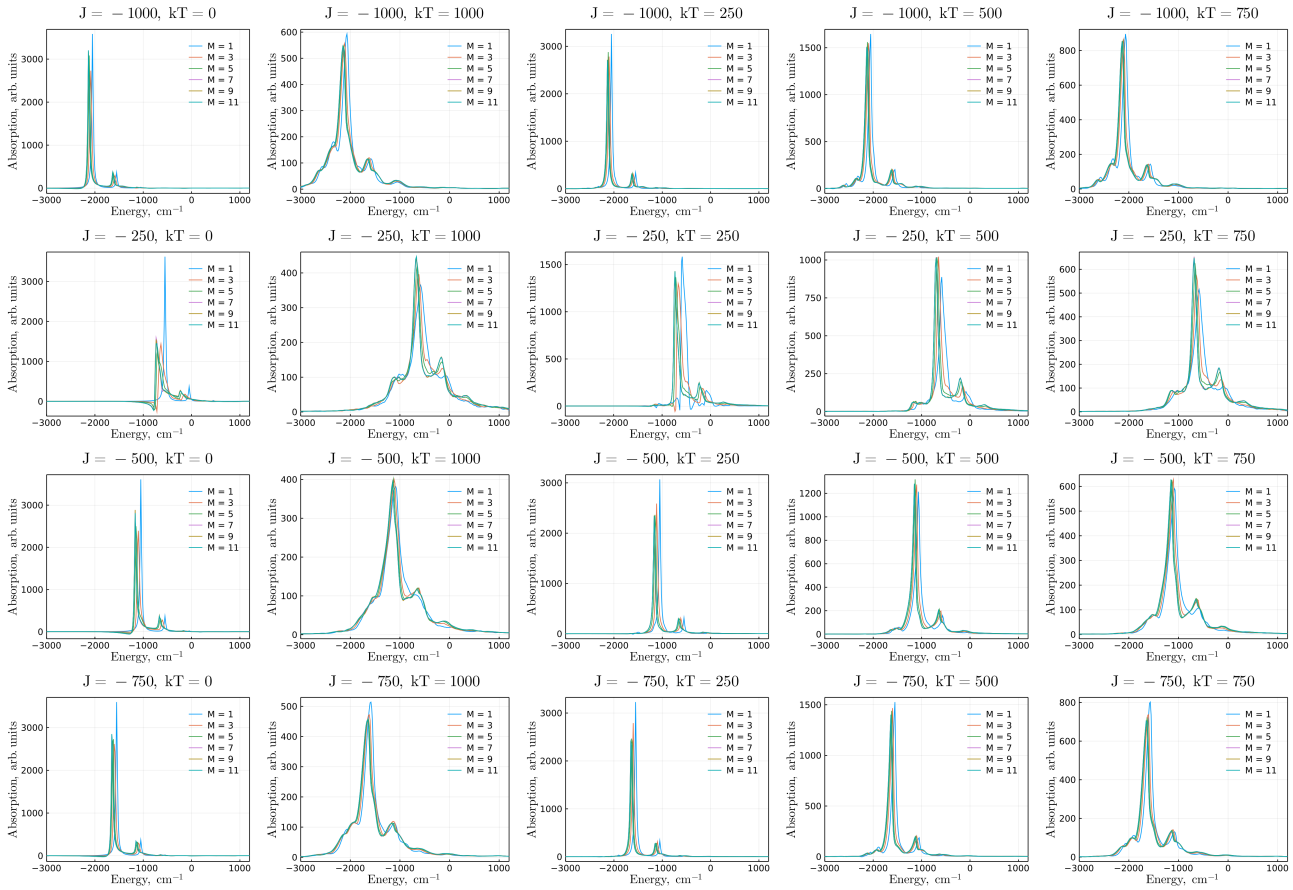

Figure 2. Absorption spectra of model J aggregate in an *closed* chain configuration, computed with mD_2 Ansatz depth M, nearest neighbor coupling J and vibrational mode thermal energy $k_\mathrm{B}T$.

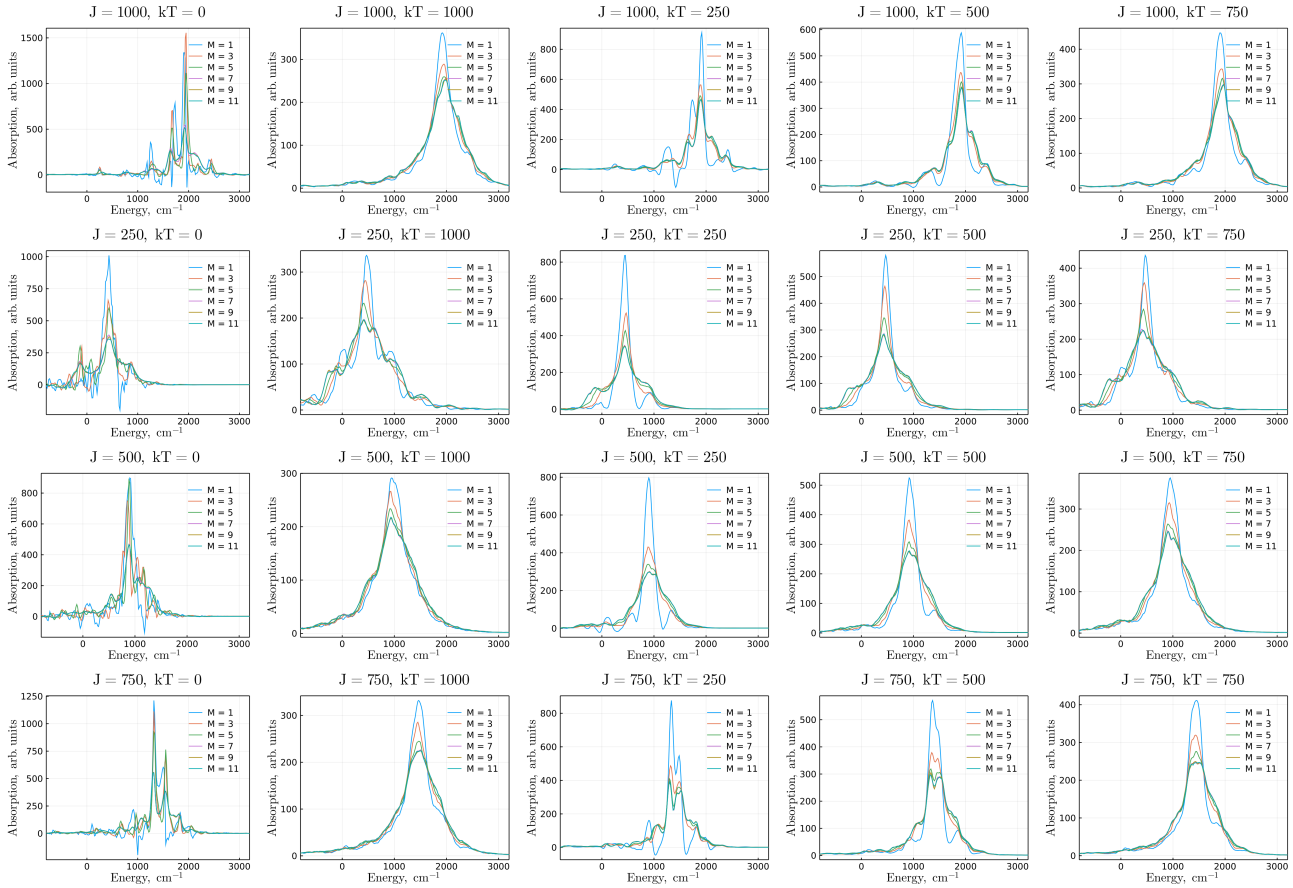

Figure 3. Absorption spectra of model H aggregate in an *open* chain configuration, computed with mD_2 Ansatz depth M, nearest neighbor coupling J and vibrational mode thermal energy $k_\mathrm{B}T$.

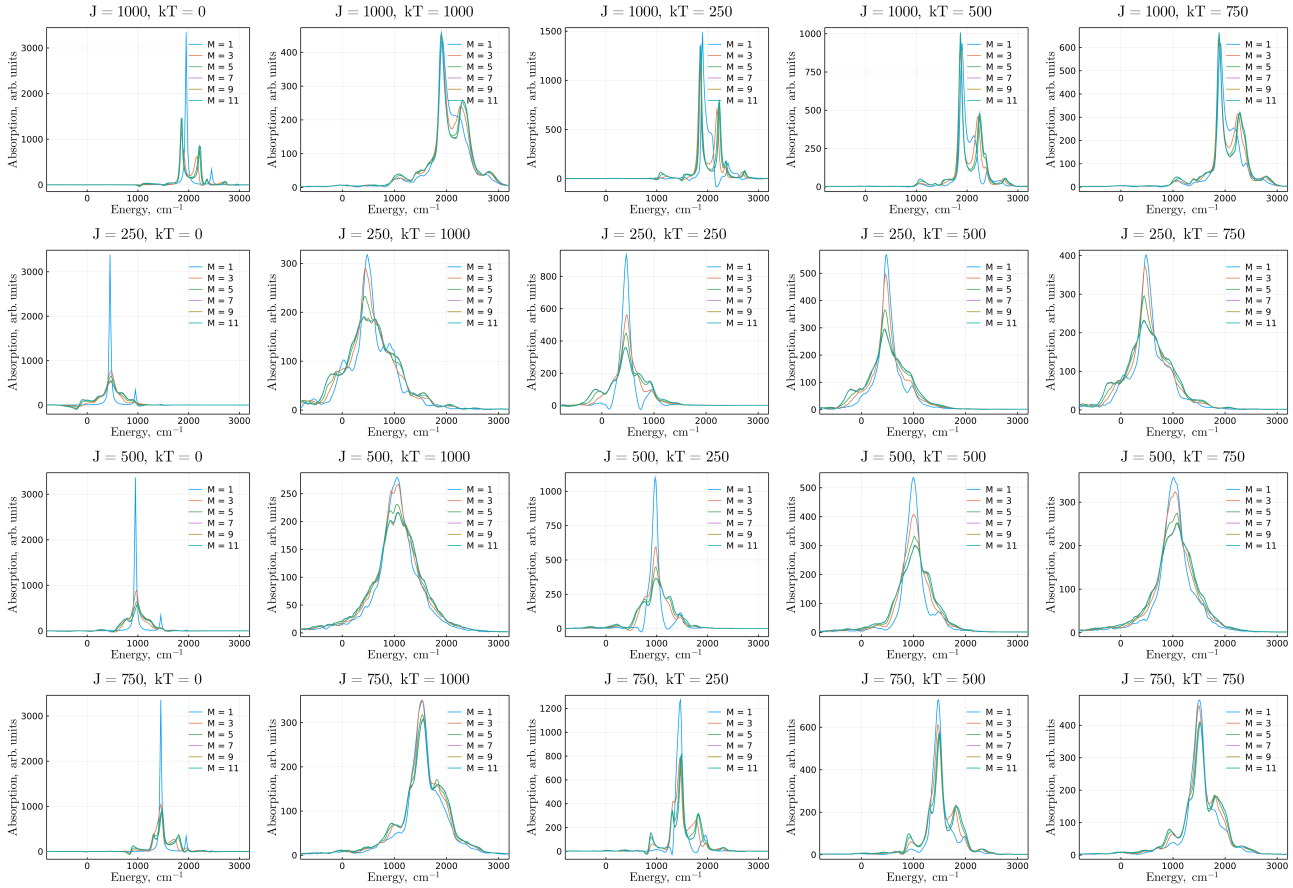

Figure 4. Absorption spectra of model H aggregate in an *closed* chain configuration, computed with mD_2 Ansatz depth M, nearest neighbor coupling J and vibrational mode thermal energy k_BT.