

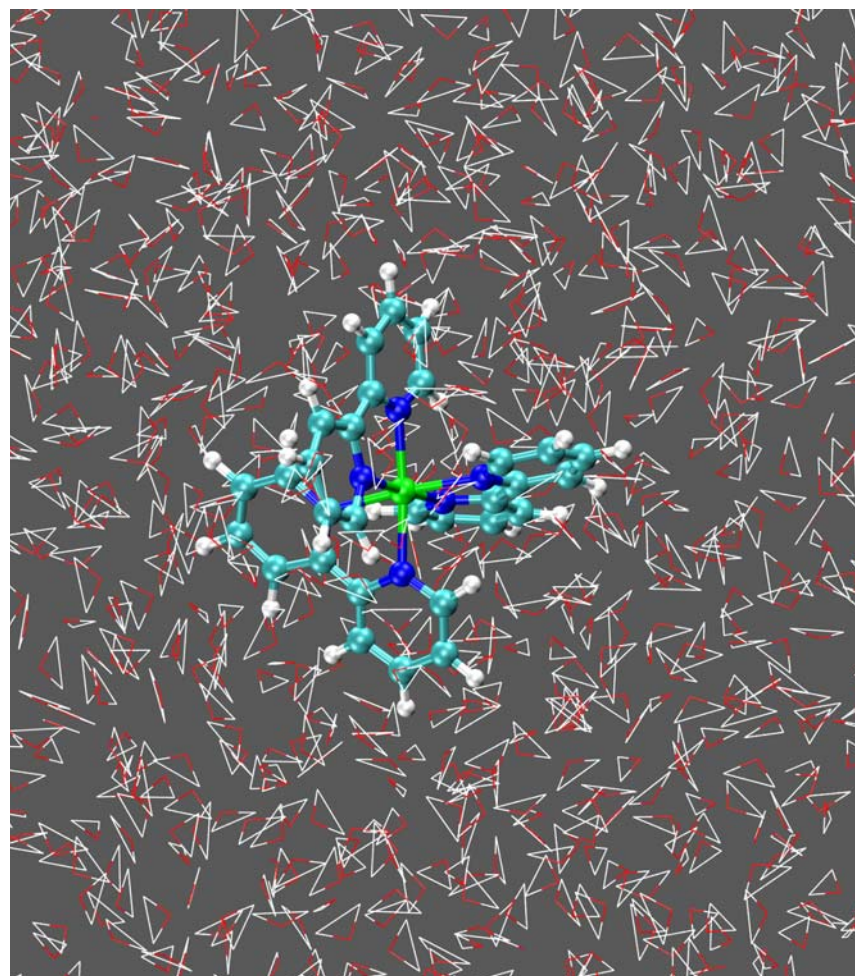
Energetics and Solvation Dynamics of the Excited $\text{Ru}(\text{bpy})_3$ Complex in Water

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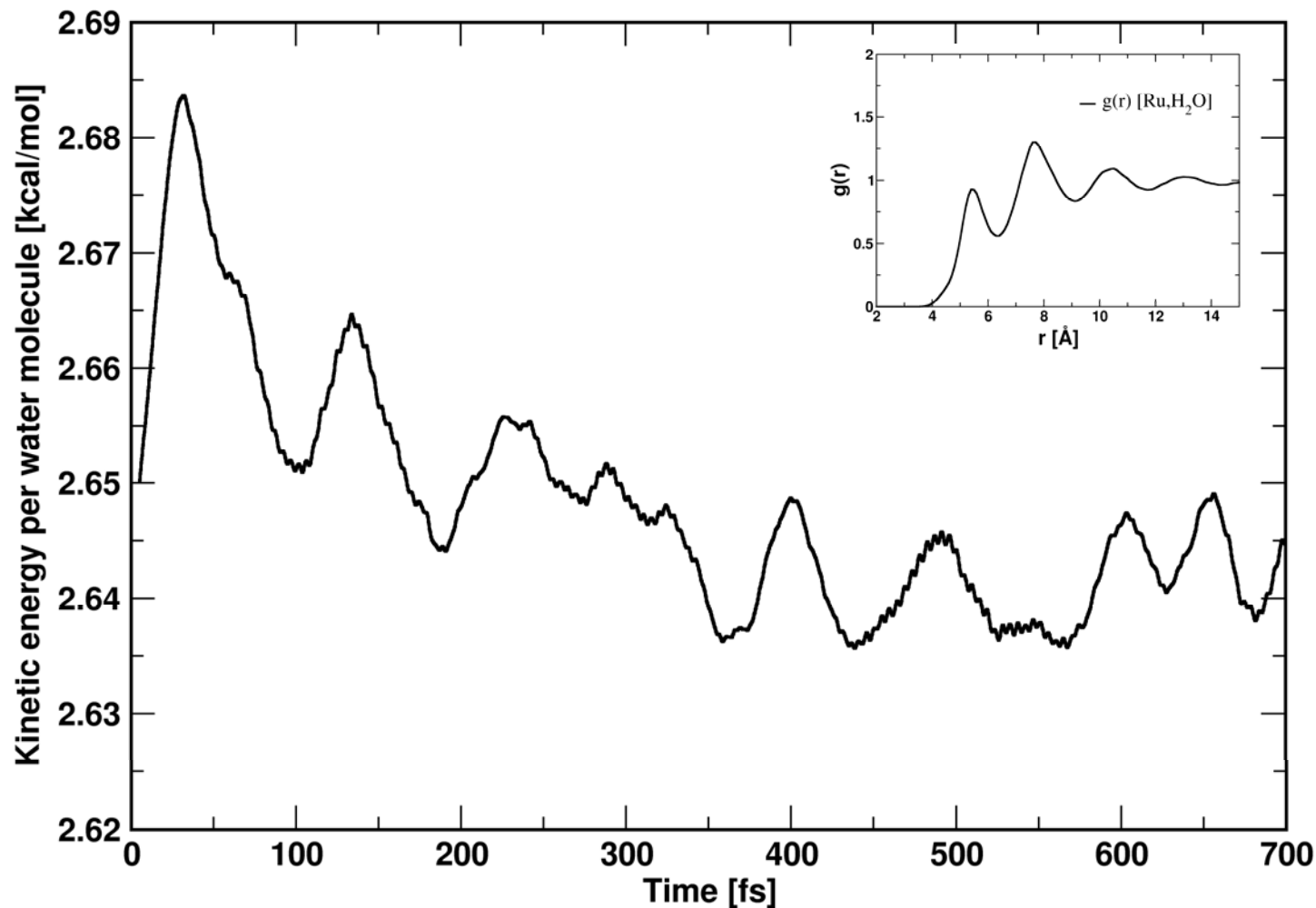
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- Compound widely used as a model in the solar-energy harvesting processes.
- Experimental data available
- Well-established theoretical model of the process
- **Question:** How solvent contributes to unusual stability of the excited state?

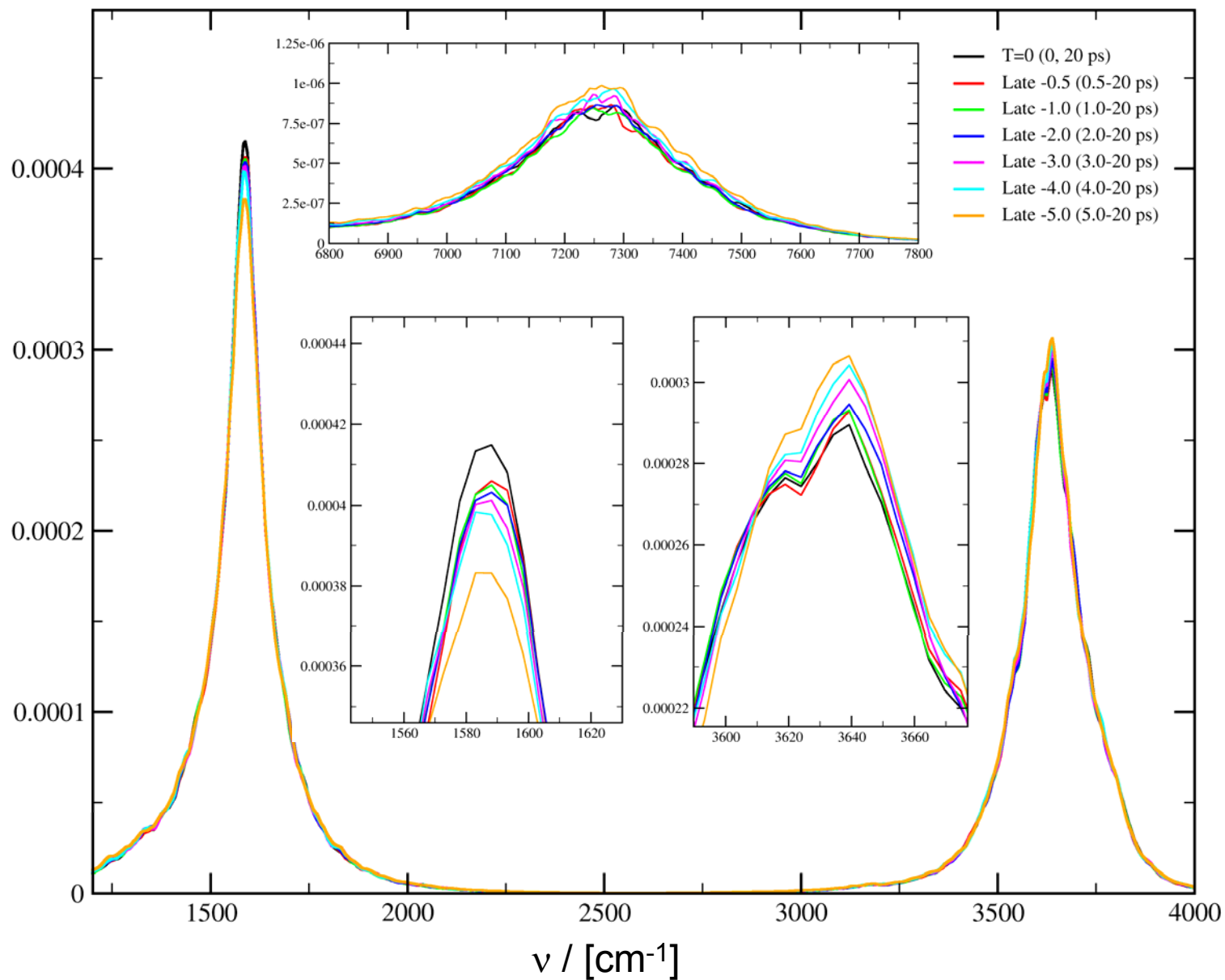


- MD simulations were carried out with VALBOND-TRANS* code implemented in CHARMM program (combined with CHARMM22 force field)
- Number of independent simulations: 100
- Time step 0.2 fs; Total time 20 ps
- Flexible water model (KKY), ~1700 waters
- Excitation modelled by switching force field* from Ru(II) to Ru(III)

*TRANS parameters taken from Tubert-Brohman *et al.*, JCTC 5, 530 (2009).



- Energy transfer to the solvent occurs within 35 fs
- Signal decays in approx. 350 fs



- VALBOND-TRANS code has been verified; excited ($^3\text{MLCT}$) state populated within ~ 300 fs (QM/MM)*
- Water assists in absorbing excess of energy after photo-excitation; importance of IVR has not been verified at this point
- Spectral signal manifestation in changes of the amplitudes rather than shift of the peak

*taken after Moret *et al.* Chem. Eur. J. 16, 5889 (2010).



Thank You