

# Screening Excited-State Dynamics in Emissive Vanadium(III) Complexes using Surface Hopping with Linear Vibronic Coupling

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The linear vibronic coupling (LVC) is an efficient method to parametrize potential energy surfaces for multiple electronic states. In combination with surface hopping (SH) it allows to simulate the photodynamics of transition metal complexes including all vibrational degrees of freedom and many close-lying electronic state on picosecond timescales. These methods can be important to guide experimental study and help the design of novel photoactive transition metal complexes. [1] First row transition metal complexes are sustainable and Earth abundant potential substitutes for photochemically active complexes based on expensive noble metals. To compensate the unfavorably small ligand field splitting and spin orbit coupling qualities of 3d metals which often induce efficient non-radiative photochemical relaxation to the ground state, ligands with special electronic properties are needed. Previous studies have shown that the strong field ligand ddpd (Figure 1) can induce phosphorescence in the  $\text{VCl}_3\text{ddpd}$  complex. [2] Photodynamics simulations of  $\text{VCl}_3\text{ddpd}$  suggested that improved emissions properties can be achieved by increasing the ligand field splitting. [3] In our work we use the SH/LVC approach to improve the photoluminescence of vanadium(III) complexes containing strong-field ligands. We identify four promising candidates for which excited-state dynamics were performed using SH/LVC with potentials parametrized from CASSCF/CASPT2 calculations. This approach revealed two complexes with improved emission properties compared to the reference  $\text{VCl}_3\text{ddpd}$ .

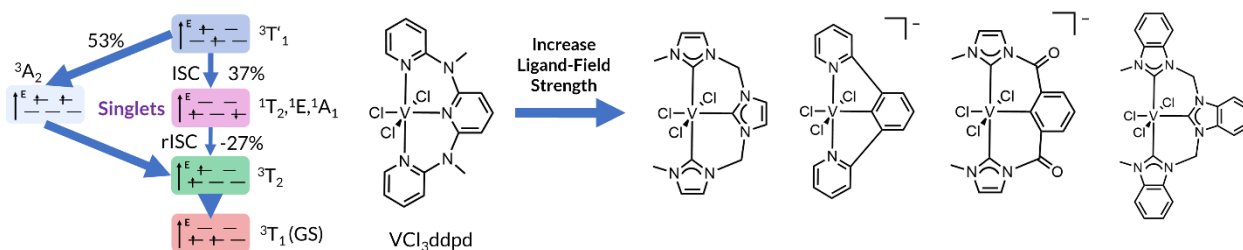


Figure 1.: Mechanism of  $\text{VCl}_3\text{ddpd}$  and candidate complexes

[1] J. P. Zobel et al.; *Acc. Chem. Res.* **54** 3760 (2021)

[2] M. Dorn et al.; *Chem. Sci.* **12** 10780 (2021)

[3] J. P. Zobel et al.; *Chem. Sci.* **12** 10791 (2021)