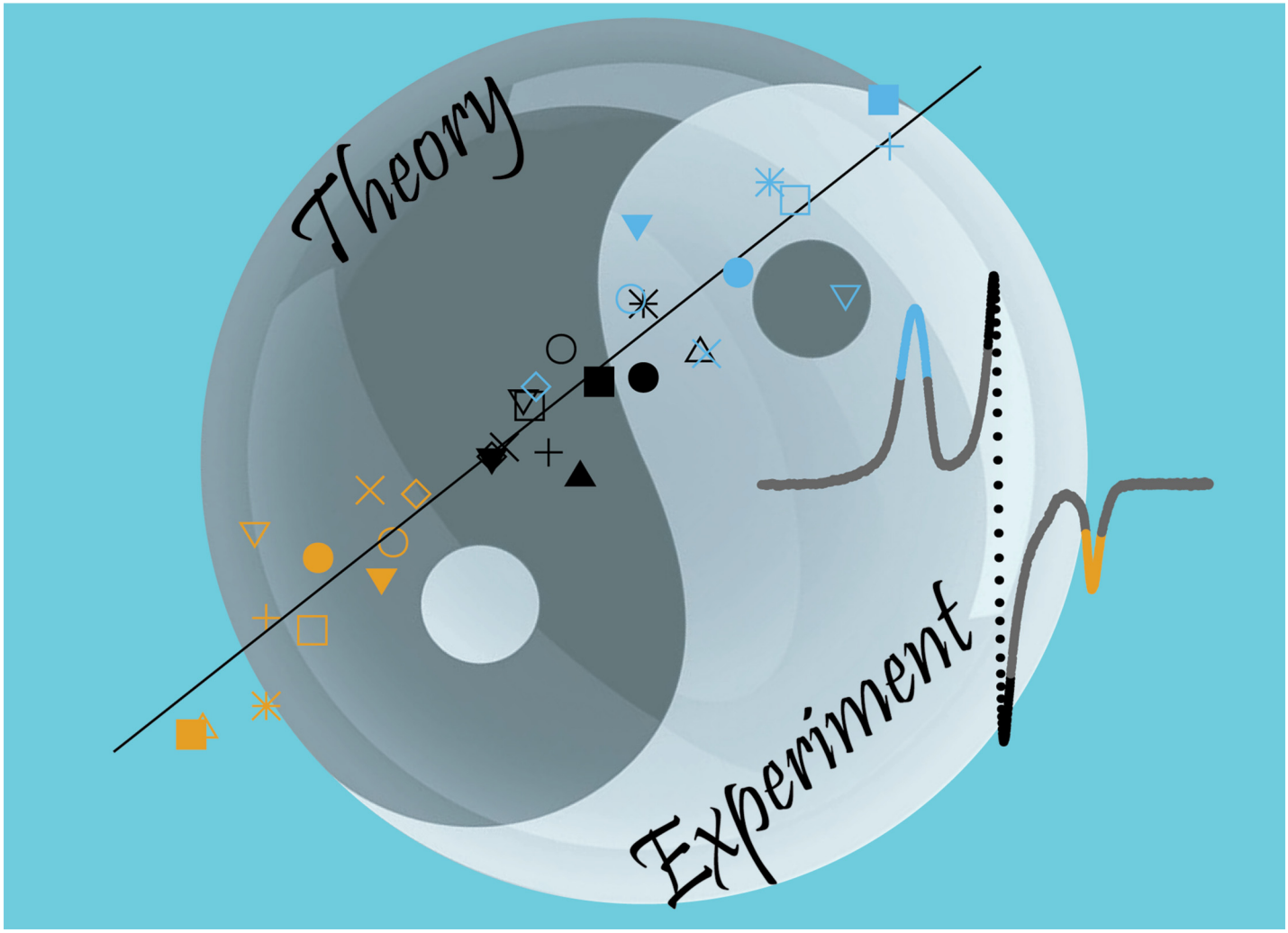

Showcasing research from Professor Pushkar's laboratory, Department of Physics and Astronomy, Purdue University

Multiconfigurational electronic structure calculations explain the role of ligands in *g*-tensor anisotropy for Ru^{III} complexes

Identification of radical intermediates by means of electron paramagnetic resonance benefits from theoretical computation of the EPR parameters such as *g*-tensor and hyperfine splitting. Here, we provide a theoretical analysis for twelve reactive Ru^{III} intermediates catalysing water oxidation, a key reaction in artificial photosynthesis. Using multireference methods, we compute *g*-tensor values and assess the errors against experimental data. Our calculations reproduce previously reported experimental trends, which we explain from a theoretical perspective. Based on our benchmarking we recommend a robust computational protocol.

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See Pavel Pokhilko and Yulia Pushkar, *Phys. Chem. Chem. Phys.*, 2025, **27**, 22937.

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