**The Road from Quantum Chemistry to Quantum Materials**

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The rapidly evolving field of quantum computing demands precise control over the superposition states of qubits. In this lecture, I will present our advancements in the calculation of singlet–triplet gaps and zero-field splitting parameters within organometallic complexes, featuring prominent transition metal ions like Cr and V.[1] These complexes hold promise as molecular qubit candidates. I will delve into the quantum chemistry methodologies that we develop, founded upon combining multireference wave functions with density functional theory.[2][3] By harnessing these methodologies, we gain unique insights into the intricate quantum behavior of these systems, shedding light on their suitability for quantum computation. Moreover, I will discuss the convergence of computation and data-driven techniques in the realm of quantum materials discovery.

[1] A. Sauza-de la Vega, R. Pandharkar, G. D. Stroscio, A. Sarkar, D. G. Truhlar, and L. Gagliardi, Multiconfiguration Pair-Density Functional Theory for Chromium(IV) Molecular Qubits, *JACS Au*, **2022**, 2, 2029–2037. DOI: 10.1021/jacsau.2c00306

[2] S. Haldar, A. Mitra, M. Hermes, and L. Gagliardi, Local Excitations of a Charged Nitrogen Vacancy in Diamond with Multireference Density Matrix Embedding Theory, *J. Phys. Chem. Lett*. *0*, **2023**, 14, 4273–4280 , DOI: 10.1021/acs.jpclett.3c00551

[3] M. Otten, M. R. Hermes, R. Pandharkar, Y. Alexeev, S. K. Gray, and L. Gagliardi, Localized Quantum Chemistry on Quantum Computers, *J. Chem. Theory Comput.*, **2022**, 18, 7205–7217. DOI: 10.1021/acs.jctc.2c00388