PHYSICAL SEMINAR

Quantum Coherence in Chemistry: Tackling the Decoherence Challenge

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To unlock the sophistication of chemistry in building complex molecular architectures to develop nextgeneration quantum technologies, there is a critical need to identify robust molecular design principles that can be used to generate quantum subspaces with protected or controllable coherences [1]. Systematic progress requires developing experimental and theoretical methods to quantify and manipulate quantum coherences and understanding how the decoherence (or quantum noise) introduced by the environment influences the system's dynamics.

In this talk, I will summarize recent efforts in my group to advance the theory, simulation and interpretation of quantum decoherence in chemistry [2-7]. Specifically, I will introduce the TTN-HEOM [2], a numerically exact method for open quantum dynamics that makes the powerful but memoryhungry hierarchical equations of motion (HEOM) practical for real-world simulations by using tree tensor networks (TTN) to compress and organize the equations. The method now enables simulations of driven quantum system interacting with highly structured environments typical of chemistry and quantum information science. I will further introduce our theory of decoherence pathways [3-7] that now enable quantifying the contributions of specific vibrations or solvent modes to the overall decoherence of molecular-based quantum subsystems. These theories provide the means to finally establish the basic chemical principles of quantum decoherence phenomena.

References

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[3] I. Gustin, C.W. Kim, D.W. McCamant, and I. Franco, *Proc. Natl. Acad. Sci. U.S.A*. **120**, e2309987120 (2023)
[4] C. W. Kim and I. Franco, *J. Chem. Phys.* **160**, 214111 (2024)
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Wednesday, November 5, 2025 **10:30 am** **BRWN 4102**

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