



**Division of Physical Chemistry
American Chemical Society**

QIS for Chemistry and Chemistry for QIS

**Ben Augenbraun
Justin Caram**
Organizers

San Diego Convention Center
see schedule for room locations

23-27 March 2025

PHYS Programs also available online:



SUNDAY MORNING

Manipulating Electron Spins for QIS
J. Zadrozny, *Presiding* | **Hall F, Room 3**

8:00 AM. Synthetic control of spin-correlated radical pairs for emissive molecular qubits. N. Lin, M. Tsuji, I. Bruzzese, A. Chen, M. Vrionides, N. Jian, F. Kittur, T.P. Fay, **T. Mani**

8:30 AM. Divacancy Graphene and Graphyne as potential biomedical sensors: A first-principles study. **M.N. Mattur**, E. Haidar, O.J. Conquest, C. Stampfl

8:50 AM. Unveiling a new regime of electron spin coherence for molecular quantum information science. **R. Hadt**

9:20 AM. Photo-induced spin polarization in MOFs and dimers. **N. Yanai**

9:50 AM. Spectrochemical series for electron spin relaxation. **N. Kazmierczak**, K.T. Xia, E. Sutcliffe, J.P. Aalto, R. Hadt

10:10 AM. Theories and driven open system quantum dynamics methods for quantum sensing. **S.J. Jang**

10:40 AM. Electron spin relaxation and decoherence dynamics in spin-labeled micelles. **C.A. Totoiu**, N. Kazmierczak, A.A. Laaj, J. Cao, R. Hadt

SUNDAY AFTERNOON

Computational Chemistry and QIS
H. P. Hendrickson, *Presiding* | **Hall F, Room 3**

2:00 PM. Simulating quantum dynamics on classical computers, quantum simulators, and real quantum hardware: a study of free particles, harmonic oscillators, and tunneling. **T. Kuanysheva**, B. Kendrick, L. Cincio, D. Babikov

2:20 PM. Non-unitary variational quantum eigensolver with the localized active space method. **Q. Wang**, R. D'Cunha, A. Mitra, Y. Alexeev, S.K. Gray, M. Otten, L. Gagliardi

2:40 PM. Quantum accelerated supercomputing for chemistry simulations. **M. Farag**

3:10 PM. Developing quantum machine learning algorithms to predict electrophilicity. **H.P. Hendrickson**, L. Boyle, S. Tadisina, C. Takahashi, V. Venkatesh, N. Vu, J. Yan, C. Yeung, D. Grace, C. Xu, V.S. Batista, S. Nkomo

3:40 PM. Modeling ATP hydrolysis on quantum hardware.

B. Rubenstein, P. Vaish, Y. Pang, C. Batton, M.s. Chen, H. Singh, W. Mullinax, N. Tubman, G. Rotskoff

4:10 PM. Fast chemical screening of Josephson junctions. **W. Xie**, C. Peng

4:40 PM. Simulating electronic structure on bosonic quantum computers. R. Dutta, **N. Vu**, C. Xu, N. Lyu, A. Soudackov, X. Dan, H. Li, C. Wang, V.S. Batista

MONDAY MORNING

QIS and Chemical Environments

J. R. Caram, *Presiding* | **Hall F, Room 3**

8:00 AM. Developing a chemical intuition for orbital specific control in lanthanide complexes. **A.B. Altman**, P. Reuel, S. Chowdhury, H. Jemison, R. O'Shea

8:30 AM. Taming molecular qubits through electronic strong coupling. **J.J. Foley**, N. Vu, R. Manderna, P. Roden, L. Tolley

9:00 AM. Leveraging metal-ligand covalency in optically-gated spin-based quantum states. **N. Frank**, S. Ghosh, P. Oyala, S.O. Odoh, E.R. Bittner

9:30 AM. Towards ultracold MgF molecules for quantum information science. **E. Chae**

10:00 AM. Clock transitions in molecular nanomagnets and solid-state defects: Pathways towards noise-resistant qubits. **J.R. Friedman**

10:30 AM. Exploring lanthanide-based single molecule magnets: insights into photon-initiated electron-neutral interactions for quantum information science applications. **L.M. Thompson**, H.P. Hratchian, C. Jarrod

11:00 AM. Computational study of spin dynamics in two pincer-type Co(II)/Cu(II) complexes. **M. Fizer**, V. Dergachev, S. Ghosh, P. Oyala, N. Frank, S.A. Varganov

WEDNESDAY MORNING

Optical State Preparation and Protection for QIS

B. Augenbraun, *Presiding* | **Room 33C**

8:00 AM. Tunable spin qubit pairs in quantum dot – molecule conjugates. **J.H. Olshansky**

8:30 AM. Alternant hydrocarbons as optically addressable molecular qubits. **J. Yuen Zhou**

9:00 AM. Theoretical design of quantum functional groups.
T. Khvorost, R.J. Choi, C. Dickerson, A. Alexandrova

9:20 AM. Quantum operations of condensed-phase ytterbium coordination complexes for field sensing. **Y. He**, C. Zhao, H. Roshandel, B.Y. Li, A.J. Shin, P. Diaconescu, W.C. Campbell, J.R. Caram

9:40 AM. Bridging topological band theory and molecular chemistry. **L. Muechler**

10:10 AM. Spin-vibronic coupling in polyatomic molecules pertinent to optical cycling efficiencies. **L. Cheng**

WEDNESDAY AFTERNOON

Synthetic Color Centers and Spin Qubits for QIS

J. H. Olshansky, *Presiding* | **Room 33C**

2:00 PM. Molecular color centers. D.E. Freedman, **C. Oswood**

2:30 PM. End-to-end quantum simulation of a chemical system.

H. Liu

3:00 PM. Quanta-Bind: A quantum computing pipeline for strongly correlated systems in metalloproteins. **T.S. Hardikar,**

J.H. Brown,

K. Heitritter, R. D'Cunha, A. Mitra, S. Weatherly, Y. Liu, M. Otten,

T.A. Van Voorhis, Y. Alexeev, L. Gagliardi, K. Setia

3:30 PM. Modeling electron spin dynamics in paramagnetic molecules with nonadiabatic molecular dynamics.

V. Dergachev, S.A. Varganov

3:50 PM. Understanding magnetic noise at the molecular level.

J. Zadrozny

THURSDAY MORNING

Manipulating Excitons for QIS

C. Chuang, *Presiding* | **Room 31C**

8:00 AM. Growth and characterization of ion-linked bilayers on MoS₂: A pathway to functional interface engineering. **A. Arcidiacono**, C.R. Johnston, C. Keenan, N. Mirzajani, A. Ghosh, A.S. Filatov, S.B. King

8:20 AM. Triplet exciton-mediated quantum chain using mixed crystals with a tailor-made triplet sensitizer. **I. Paul**

8:40 AM. Detecting entanglement in open vibronic systems via the Cauchy-Schwarz inequality. N. Jacobus, P.W. Brumer, **C. Chuang**

9:10 AM. Disorder enhanced exciton transport and quantum information spreading with the assistance of cavity QED. **W. Wu**, A.N. Hejazi, G.D. Scholes

9:30 AM. Analyzing non-Markovian quantum dynamics from quantum information perspective. **F. Wang**

10:00 AM. Singlet fission for quantum information science: Can we predict triplet pair spin evolution?. M. Collins, D. McCamey, **M. Tayebjee**

The organizers acknowledge the following sponsors for their generous support:

