Division of Physical Chemistry
American Chemical Society

Prospects of Quantum Computing for Quantum Chemistry

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Organizers

Walter E. Washington Convention Center
Hall E, Room 26

18-20 August 2025

PHYS Programs also available online:

MONDAY MORNING

Embedding & Early Fault-Tolerant Quantum Computing Methods

S. Knecht, *Presiding*

8:00 AM. Quantum computation of molecular recognition. **M. Reiher**

8:30 AM. Intermission.

8:35 AM. Alchemical free energy calculation using quantum hardware. **Z. Li**, D. Kaliakin, A. Shajan, M. Bazayeva, F. Liang, S. Das, K.M. Merz

8:55 AM. Intermission.

9:10 AM. Dynamical mean field theory for real materials on a quantum computer. **M. Amsler**, J. Selisko, C. Wever, G. Samsonidze, Y. Kawashima, R. Haq, F. Tacchino, I. Tavernelli, T. Eckl

9:40 AM. Intermission.

9:45 AM. Quantum simulation of carbon capture in periodic metal-organic frameworks. **P. Ollitrault**, J. Gonthier, R. Parrish, T. Schäfer, A. Grüneis, B. Kang, H. Lee

10:05 AM. Intermission.

10:20 AM. End-to-end simulation of a chemical system with reliable quantum computing. **W. van Dam**

10:50 AM. Intermission.

10:55 AM. Simulating vibrational Hamiltonians on a quantum computer using Trotter product formulas. **S. Malpathak**, S. Kallullathil, I. Loaiza, S. Fomichev, J. Arrazola, A.F. Izmaylov

11:15 AM. Intermission.

11:30 AM. Challenges and opportunities for chemical simulation on early fault-tolerant quantum processors. **W.J. Huggins**

MONDAY AFTERNOON

Sample-Based Quantum Diagonalization Methods & Applications

T. P. Gujarati, *Presiding*

2:00 PM. Electronic structure beyond the scale of exact diagonalization on a quantum-centric supercomputer. **P. Jurcevic**

2:30 PM. Intermission.

3:30 PM. Computational chemistry enabled by quantum computers. **K.M. Merz**

4:00. PM. Intermission.

4:30 PM. Improved sample-based quantum diagonalization via randomized Hamiltonian simulation. S. Piccinelli, **M. Rossmannek**

4:50 PM. Intermission.

5:00 PM. Quantum-centric study of methylene singlet and triplet states. **K. Doney**

5:30 PM Intermission.

5:40 PM. Hybrid quantum-classical simulation of periodic materials. **R. Neumann Barros Ferreira**, A. Duriez, P. Costa Carvalho, M. Barroca, F. Zipoli, B. Jaderberg, T. Reschützegger, K. Sharma, A. Mezzacapo, B. Wunsch, M. Steiner

TUESDAY AFTERNOON

Variational Quantum Algorithms & Beyond

P. Ollitrault, *Presiding*

2:00 PM. Scaling quantum chemistry on quantum computers: An end-to-end perspective. **S. Knecht**

2:30 PM. Intermission.

2:40 PM. Variational quantum annealing for quantum chemistry. K. Yip, K. Yeter-Aydeniz, **S.S. Dong**

3:00 PM. Intermission.

3:15 PM. Local subspace variational quantum compilation for large-scale Hamiltonian simulation. **S. Kanasugi**, Y. Hidaka, Y.O. Nakagawa, S. Tsutsui, N. Matsumoto, K. Maruyama, H. Oshima, S. Sato

3:45 PM. Intermission.

4:15 PM. Qubit-efficient quantum chemistry with the ADAPT variational quantum eigensolver and double unitary downfolding. **H. Singh**, N. Mayhall, L. Bertels, D. Chaves Claudino, S. Economou, E. Barnes, N.P. Bauman, K. Kowalski

4:35 PM. Intermission.

4:50 PM. Molecular excitation energies simulated on a superconducting quantum computer. **F. Pavosevic**

5:20 PM. Intermission.

5:30 PM. Unleashed from constrained optimization: Quantum computing for quantum chemistry. **B. Peng**

WEDNESDAY AFTERNOON

Ansatz Design & State Preparation

M. Rossmannek, *Presiding*

2:00 PM. Rethinking electronic wavefunction theory for quantum computation. **H.G. Burton**

2:30 PM. Intermission.

2:40 PM. Reducing the quantum resource requirements for simulating molecules: Generalized entanglement forging. **T.P. Gujarati**, I. Liepuoniute, M. Motta, T. Friedhoff, T. Smith, B. Link, N. Nguyen, H. Nishimura, K. Williams

3:00 PM. Intermission.

3:15 PM. Enhancing initial state overlap through orbital optimization for faster molecular electronic ground-state energy estimation. **P. Ollitrault**, C. Cortes, J. Gonthier, R. Parrish, D. Rocca, G. Anselmetti, M. Degroote, N. Moll, R. Santagati, M. Streif

3:45 PM. Intermission.

4:15 PM. Quantum-classical auxiliary field quantum Monte Carlo with Matchgate shadows on trapped ion quantum computers. **L. Zhao**, **J. Goings**, E. Epifanovsky, M. Roetteler

4:35 PM. Intermission.

4:50 PM. Generative quantum eigensolver in the age of AI for Quantum computing. **K. Nakaji**

5:20 PM. Intermission.

5:30 PM. Constrained nuclear-electronic orbital theory for quantum computation. **T. Culpitt**, Y. Yang