Machine learning meets electronic structure theory

Organizers: Yeongsu Cho and Fang Liu August 24-26, 2026

Monday AM

McCormick Place Convention Center W180
Y. Cho, F. Liu, *Organizers* | F. Liu, *Presiding*

8:00 AM. Multireference methods and foundational models for chemistry and materials. **L. Gagliardi**, A. Seal, H.S. Clifford

8:35 AM. Nonlocal machine-learned density functionals for Materials Chemistry. **K. Bystrom**, M. Abdallah, Z. Jin, B. Kozinsky

8:50 AM. Machine learning the two-electron reduced density matrix in molecules and condensed phases. **M. Pavanello**, J. Martinez, B. Rana, X. Shao, K. Pernal

9:25 AM. Automating density matrix embedding theory with weighted active space Protocol. **T. Strang**, A. Seal, S. Verma, L. Gagliardi

9:40 AM. Intermission.

10:05 AM . graphpancake: a Python package for representing organic molecules as molecular graphs utilizing electronic structure theory. **S. Sil**, M.A. Maskeri, K. Scheidt

10:20 AM. Understanding the thermodynamics of BeF_2 through machine learning accelerated density functional theory calculations. **P. Wisesa**, J. Paz Soldan Palma, J. Schorne-Pinto, T.M. Besmann

10:35 AM. CAS-ESM: A multireference electronic structure-aware surrogate model for transition metal catalysis and excited state dynamics. **A. Seal**, B. Jangid, A. Ferguson, L. Gagliardi

10:50 AM. Data-driven quantum chemistry for geometry optimization and strong electron correlation. **K.D. Vogiatzis**

11:25 AM. Controlled cloning of exchange–correlation functionals: toward physically grounded ML-DFT. **M. Fernandez-Serra**

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Monday PM

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2:00 PM. Energy and forces are all you need. **B. Cheng**

2:35 PM. Neural-network force fields for protein--ligand interactions based on energy decomposition analysis. **J.M. Herbert**, N. Puthillathu, M.L. Gray

2:50 PM. Hybrid machine learning / physics based models of intermolecular interactions. **C.D. Sherrill**

3:25 PM. Spin differentiation in machine learning interatomic potentials for broken-symmetry solution. **B. Kalita**, R. Zubatyuk, O. Isayev

3:40 PM. Intermission.

4:00 PM. Transferable FB-GNN-MBE framework for potential energy surfaces: A teacher–student pipeline in deep-learned many-Body expansion theory. **Z. Lin**

4:35 PM. Ultra-fast universal machine learning interatomic potential based on Deep Sets. **C.A. Kim**, J.L. Bjorklund, S.E. Mason, X. Qu

4:50 PM. From electrons to reactions: Machine learning potentials with neural spin-charge equilibration for reactive chemistry. **O. Isayev**

5:25 PM. Making general-purpose ML force fields reliable: Atom-centered labeling for chemical space coverage and extrapolation detection. **I. Poltavskyi**

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Tuesday AM

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8:00 AM. Introductory Remarks.

8:05 AM. Accelerating high-accuracy transition state optimization via a PCA-driven multi-fidelity workflow. **S. Nirenberg**, Y. Liu, B. Rubenstein

8:20 AM. Accelerating variational quantum computing workflows for defect containing condensed matter studies via inter- and intra-structural parameter transfer: Applications to battery cathode. **S. Shivpuje**, V. Singh, P. Mlkvik, M. Sajjan, M. Farag, N. Spaldin, S. Kais

8:35 AM. Domain-informed representations and architectures for machine-learning electronic structure properties of transition-metal complexes. **I. Kevlishvili**

9:10 AM. From small datasets to large language models - Challenges and opportunities in data-driven material design. **J. Wang**

9:45 AM Intermission.

10:05 AM. LLM-guided symbolic regression for wavefunction-informed exchange-correlation functional development. **V. Khanna**, H. Cai, J. Kammeraad, P.M. Zimmerman

10:20 AM. Prospect of chemically transferable electronic coarse-graining models. **N. Jackson**

10:55 AM. Accelerated discovery of multicomponent alloys via machine learning and electronic structure theory. **H. Qin**, Q. Zhao

11:10 AM. Hamiltonian prediction across the periodic table. **D.S. Levine**, M. Kaniselvan, B.K. Miller, M. Gao, J. Nam

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2:00 PM. Accelerating the prediction of the electronic and coherent properties of spin qubits in solids and molecules using machine-learning and data-driven strategies. **G.A. Galli**

2:35 PM. Accurate core-level spectroscopies from machine learned potential architectures. **D. Hait**, P. Pope, B. Shi

2:50 PM. Machine learning framework for mean-field and many-body effective Hamiltonians. **T. Zhu**, C. Zhang, C. Venturella

3:25 PM. Super-resolution methods for accelerating large-scale electronic structure calculations. A. Gorfer, T.A. Van Voorhis, K.U. Reuter, **M. Kick**

3:40 PM. Intermission.

4:00 PM. Machine learning meets multiscale models: spectroscopic properties and excited-state dynamics in condensed phase. **L. Cupellini**

4:35 PM. Machine learning of ground- and excited-state electronic structure. **B. Rana**, J. Martinez, M. Pavanello

4:50 PM. MBFormer: A general machine learning framework for many-body interactions in real materials. **D.Y. Qiu**

5:25 PM. Quantum dynamics of electronic excitations with machine learning. **O.V. Prezhdo**

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Wednesday AM

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8:35 AM. From symmetry discovery to active learning: Machine learning workflows for first principles electrocatalysis on disordered materials. **O. Andreussi**

8:50 AM. Intermission.

9:25 AM. Data-driven transition state discovery via machine-learned potentials and string methods. **J. Gomes**

9:40 AM. Intermission.

10:00 AM. High-throughput design of materials via low-scaling calculations and the automated workflow. **J. Ma**

10:35 AM. Modeling biochemistry on quantum hardware: a marriage of machine learning, electronic structure, and quantum algorithms. **B. Rubenstein**, P. Vaish, Y. Pang, E. Ivaniashvili

10:50 AM. Inverse computational design of conjugated molecules and oligomers. **D.P. Tabor**

11:25 AM. Environment-aware machine learning approaches for the design of macromolecular photoredox catalysts. **S.S. Dong**

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2:00 PM. Introductory Remarks.

2:05 PM. Composition-dependent oxygen vacancy mechanisms in layered oxides revealed by machine learning residuals and electronic structure analysis. **S.E. Mason**, J.L. Bjorklund, D. Fennell

2:20 PM. Direct variational calculation of two-electron reduced density matrices *via* semidefinite machine learning. **L.H. Delgado**, D.A. Mazziotti

2:35 PM. Toward the exact exchange-correlation functional: A neural network construct. **G. Chen**

3:10 PM. Quantum machine learning through hybrid quantum-neural molecular wavefunction. **Z. Shuai**

3:45 PM. Intermission.

4:00 PM. Tale of two splines: towards next-generation density functionals and machine learning for chemistry. **R.A. Distasio**

4:35 PM. Deep-learning DFT Hamiltonians for efficient electronic structure calculations. **Z. Tang**, W. Duan, Y. Xu

5:10 PM. Machine-learning augmented electronic structure calculations via adaptive DFTB parameters. **Y. Song**, A. Samtsevych, C. Scheurer, K.U. Reuter, C. Panosetti

5:25 PM. Linear-scaling orbital-free density functional theory *via* Fourier neural operators. **D. Khan**, M. Hanisch, A. Anandkumar

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