Division of Physical Chemistry
American Chemical Society

Embedding Methods for Ground and Excited States

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Organizers

Walter E. Washington Convention Center
see schedule for room locations

19-21 August 2025

PHYS Programs also available online:

TUESDAY MORNING

Classical Embedding: QM/MM

Room 152B | M. Pavanello & W. Glover, *Presiding*

8:30 AM. Introduction.

8:35 AM. Embedding models for computational spectroscopy: from solvated systems to plasmonic nanostructured materials. **C. Cappelli**

9:05 AM. Microsolvation determines the photophysics of a fluorescent DNA-protein photo-crosslinking model. **G. Iuzzolino**, F. Perrella, M. Valadan, C. Altucci, A. Petrone, N. Rega

9:25 AM. Excited state simulations of p-DAPA and mGrape fluorophores in explicit solvent. **A. Walker**

9:55 AM. Break.

10:15 AM. Using multiscale molecular modeling for rational mutagenesis in photosynthetic proteins. **L.V. Slipchenko**

10:45 AM. Microsolvation effects on conformational dynamics, NMR and Raman spectra of Bis-(thio)carbohydrazones in a non-protic solvent. F. Santoro, V. D'Amore, D. Rogolino, A. Carotenuto, L. Marinelli, D. Brancaccio, **G. Donati**

11:05 AM. Adaptive-partitioning multilayer models for dynamics simulations: QM/QM and QM/MM embeddings with on-the-fly relocating interlayer boundaries. B. Westheimer, J. Roma, A. Tran, E. Guidez, **H. Lin**

11:35 AM. Structure of the solvated electron in 1-butyl-1-methyl-pyrrolidinium dicyanamide ionic liquid. **H.H. Nguyen**, K. Huber, B. Borah, D. Das, J.F. Wishart, D.A. Blank, C.J. Margulis

TUESDAY AFTERNOON

QM/MM, Implicit Solvation, & Energy Decomposition Analysis

Room 151A | T. Zhu & M. Caricato, *Presiding*

2:00 PM. QM/MM embedding for solvent-supported electronic states.
W.J. Glover

2:30 PM. Embedded many-body perturbation theory based on generalized Poisson equation for solvated systems.
S. Kim

2:50 PM. Unraveling noncovalent interactions in complex environments. **Y. Mao**

3:20 PM. Multistate energy decomposition analysis for hydrogen bonding interactions in excited states. **J. Gao**

3:50 PM. Break.

4:10 PM. Importance of electrostatics and charge transfer for microdroplet chemistry and emulsion stability. **T.L. Head-Gordon**

4:40 PM. Continuum and multiscale approaches for wet electrified interfaces. **O. Andreussi**

5:10 PM. Non-periodic boundary conditions at surfaces of generalized cavities in efficient hybrid implicit-explicit solvation models. **G. Amante**, N. Rega

5:30 PM. Combining QM and QM/MM with machine learning and AI tools for applications in biophysics.
B. Brooks, M. Amin, F. Samarjeet, M.R. Jones, P.S. Hudson

WEDNESDAY MORNING

Fragmentation & Machine Learning

Room 151A | W. Glover & A. Walker, *Presiding*

8:00 AM. Open-source framework for fragment-based quantum chemistry. **J. Herbert**, D.R. Broderick, P. Bowling

8:30 AM. Density-based many-body expansion for proteins and protein-ligand complexes. **C.R. Jacob**

9:00 AM. Machine learning models using the one-electron reduced density matrix for ground and excited electronic states. **B. Rana**, M. Pavanello

9:20 AM. “Cluster-in-molecule” local correlation methods for large molecules and periodic systems. **S. Li**

9:50 AM. Break.

10:10 AM. Data-driven many-body embedding for biomolecules. R. Zhou, E.F. Bull-Vulpe, **F. Paesani**

10:40 AM. Size-transferable prediction of excited state properties for molecular assemblies with machine-learned exciton model. F. Ren, X. Chen, **F. Liu**

11:10 AM. Machine learning the correlated two-electron reduced density matrix (2-cRDM). **J. Martinez**, B. Rana, X. Shao, M. Pavanello

11:30 AM. Recent developments and applications of QM/MM-ML methods. **Q. Cui**

WEDNESDAY AFTERNOON
QM/QM Embedding

Room 156 | M. Caricato & M. Pavanello, *Presiding*

2:30 PM. Density functionalized QM/MM delivers chemically accurate solute-bulk solvent interactions. J. Martinez, X. Chen, X. Shao, M. Riera, O. Andreussi, F. Paesani, **M. Pavanello**

3:00 PM. Linear-scaling coupled cluster for surface chemistry and molecular solids. **H. Ye**

3:30 PM. On the entanglement of chromophore and solvent orbitals. **Y. Shao**, X. Ji, Z. Pei, J. Yang, B. Wang, Y. Mao

4:00 PM. Break.

4:20 PM. Consistent wavefunction-in-wavefunction embedding: A perspective from coupled cluster and many-body perturbation theory. **M.P. Head-Gordon**

4:50 PM. From wavefunction/DFT embedding to black-box multi-level local coupled-cluster. **J. Neugebauer**

5:20 PM. Green's function quantum embedding with local natural orbitals. **T. Zhu**, C. Venturella, J. Li

THURSDAY MORNING

Quantum Embedding

Room 151A | J. Martinez & B.Rana, *Presiding*

8:00 AM. Löwdin embedding approach for construction of frequency-dependent electron-hole interaction kernel.
A. Chakraborty

8:30 AM. Modified coupled cluster methods as impurity solvers in dynamic mean-field theory. **C. Zhang**, T. Zhu

8:50 AM. Interacting-Bath dynamical embedding for capturing nonlocal electron correlation in solids. **J. Li**, T. Zhu

9:10 AM. Intermission.

9:30 AM. Simulating absorption spectra using EOM-CCSD with a polarizable force field: Application to the GFP chromophore.
M. Caricato

10:00 AM. Static quantum embedding theory based on the coupled cluster method. **A. Shee**, M.P. Head-Gordon

10:20 AM. Tensor hypercontraction for ab initio quantum embedding methods. **J. Yang**, G. Chan

The organizers acknowledge the following sponsor for their generous support:

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