Sessions of Interest to Gaussian Users

ACS Spring 2024 Conference, New Orleans, March 17 - 24

Sunday, March 17 | Talks

Time	Title	Presenter	Room
8:00 - 8:20	Beyond Zero-sum density functional theory: Progress and prospects	Benjamin Janesko	R04
9:30 - 9:45	A many-body perspective on proton polarization in solution	Xiaosong Li	R07
10:15 - 10:35	Atom-centered density matrix propagation (ADMP) with post-Hartree-Fock accuracy: Computational improvements …	Srinivasan Iyengar	R06
10:20 - 10:40	Natural Diels-Alderase employing iminium catalysis	Kendall Houk	340
10:50 - 11:25	Computational studies of molecular machines	Kendall Houk	344
2:30 - 3:00	Real-time nuclear-electronic orbital theory	Xiaosong Li	R07
3:40 - 4:00	Sustainable approaches towards squaraine dyes with specific photoluminescence properties	Benjamin Janesko	341

Monday, March 18 | Talks

Time	Title	Presenter	Room
8:40 - 9:00	Modeling catalyzed reactions on metal-doped amorphous silicates: The case of niobium-catalyzed ethylene epoxidation	Marco Caricato	R02
10:05 - 10:35	Higher-order ambimodal cycloadditions	Kendall Houk	R04
10:35 - 11:05	Accurate pKa evaluations for complex bio-organic molecules in aqueous media	Krishnan Raghavachari	R04
11:30 - 11:45	Insight of hydrogen atom and proton transfer reactions through ab initio path integral molecular dynamics and real-time …	Jingjing Zheng	R05
11:35 - 12:00	Understanding covalency and magnetism in Ln^{3+} doped CrI_3	Xiaosong Li	R07
2:30 - 3:00	Coupling between vibronic, environmental, and electronic degrees of freedom in simulations of optical spectroscopy	Christine Isborn	R05
2:30 - 3:00	Charge migration probed by strong fields ionization: Time dependent configuration interaction and vibrational wavepacket …	H. Bernard Schlegel	R04
3:30 - 4:00	Exploring photon-initiated electron-neutral interactions in strongly correlated lanthanide complexes	Hrant Hratchian	R04
3:55 - 4:15	Controlling dynamic motion in macrocyclic molecular hinges using steric congestion as probed with variable temperature …	Benjamin Janesko	212
5:10 - 5:35	Latent space-assisted protein sampling and assessment	Peng Tao	R03
5:20 - 5:50	Derivation and implementation of the optical rotation tensor for chiral crystals	Marco Caricato	R04

Monday, March 18 | Poster Session, 12:00 – 2:00 PM, Hall C

Title	Presenter
Predicting asphaltene and bio-asphaltene ensemble X-ray absorbance spectra by coupling DFT simulation with single-molecule imaging datasets	Benjamin Janesko
Constructing a database of asphaltenes: Quantum chemistry used to contextualize single-molecule experiments within the ensemble properties …	Benjamin Janesko

Tuesday, March 19 | Talks

Time	Title	Presenter	Room
8:45 - 9:15	Adventures in strong correlation	Gustavo Scuseria	R01
4:00 - 4:20	What spin-orbit coupling approximations yield accurate actinide spectroscopy?	Xiaosong Li	206
5:05 - 5:35	Award Address: Achieving coupled cluster accuracy at DFT cost: Novel ideas from molecular fragmentation, error cancellation...	Krishnan Raghavachari	R01

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Tuesday, March 19 | Poster Session, 7:00 – 9:00 PM, Hall C

Title	Presenter
Coherent vibrational wavepacket dynamics: Advancing our understanding for the role of molecular vibrations in photochemical reactions	Xiaosong Li
Highlighting potential challenges in time-dependent equation-of-motion coupled-cluster theory	Xiaosong Li
Induced spin symmetry breaking with constrained SCF methods and its effects on symmetry restoration	Hrant Hratchian
Influence of explicit solvent environments on band gap and excitation energy statistics for the anionic GFP chromophore	Christine Isborn
Møller—Plesset second-order and double-hybrid density functional theory for accurate transition dipole moments and oscillator strengths…	Hrant Hratchian
New generation of diagonal and non-diagonal self-energies for calculations on anions: Benchmarks and applications	Joseph Vincent Ortiz
Predicting pKas of flexible polybasic pyclen derivatives: A pKa challenge	Benjamin Janesko
Transferability of intrinsic reaction coordinates between related reactions	Edward Brothers & Michael Frisch

Wednesday, March 20 | Talks

Time	Title	Presenter	Room
9:10 - 9:30	Motivating mastery of physical chemistry through problem solving and project work	James Foresman	R08
10:35 - 10:55	Computational chemistry assisting the identification of polymers	Carl Salter	R08
2:40 - 3:00	Perturbative treatment of 4-component Hamiltonians via state interaction	Xiaosong Li	R01
3:00 - 3:20	Cluster model simulations of metal-doped amorphous silicates for heterogeneous catalysis	Marco Caricato	236
4:40 - 5:00	Chemical structure database for asphaltenes and bio-asphaltenes: Linking single-molecule imaging to ensemble experiments …	E. Brothers & B. Janesko	223
4:40 - 5:00	Construction of one-electron reduced density matrices from electron densities within finite basis sets	Viktor Staroverov	R01
4:55 - 5:15	Insights on the efficient intersystem crossing of Thiosquarines: A spin-vibrational perspective	Xiaosong Li	218
5:05 - 5:25	Constructing a solute-solvent force field from ab initio calculations for spectral lineshape prediction: A cresyl violet story	Christine Isborn	R02

Wednesday, March 20 | Poster Session, 7:00 – 9:00 PM, Hall C

Title	Presenter
Enzymatic benzofuranoindoline formation in the biosynthesis of the strained bridgehead bicyclic dipeptide (+)-Azonazine A	Kendall Houk

Thursday, March 21 | Talks

Time	Title	Presenter	Room
9:00 - 9:15	Investigating intramolecular charge transfer in benzoyl pyrazinium organic salts	Hrant Hratchian	R02
9:30 - 9:45	Structure prediction for sequence-defined polymers for electron transfer	Pragya Verma	R02
10:40 - 11:00	Condensed phase optical absorption and emission spectra: Comparison of trajectory-based correlation function and …	Christine Isborn	R04