# SESSIONS OF INTEREST ( TO GAUSSIAN USERS

#### Sunday, March 23

Time	Type	Title	Presenter & Co-Authors	Location
11:00 AM - 11:20 AM T	Talk	Understanding and predicting reaction selectivities	Kendall Houk, Qingyang Zhou, Fengjiao Liu, Sebastian Richter	Hall G/H Room 6
3:35 PM - 3:55 PM T	Talk	Development of models to explore photon-initiated electron-neutral interactions in strongly correlated lanthanide complexes	Hrant Hratchian, Lee Thompson, Caroline Chick Jarrold	Room 29B
3:45 PM - 4:25 PM T	Talk	Computational studies of amphidynamic materials	Kendall Houk, Jing-Ran Shan	Room 30D

## Monday, March 24

Time	Type	Title	Presenter & Co-Authors	Location
11:15 AM - 11	:45 AM Talk	Four-current real-time methods for simulating chirality-induced spin selectivity	Xiaosong Li	Room 33B
12:00 PM - 2	2:00 PM Poster	Determination of the phase diagram of complex coacervating systems with the addition of a charged dye using molecular dynamics	Brianna Endy, James Foresman	Hall B2/C
8:00 PM - 10	):00 PM Poster	First principles simulations of optical rotation of chiral molecular crystals	Emmanuel Forson, Taylor Parsons, Marco Caricato	Hall B2/C
8:00 PM - 10	):00 PM Poster	Comparison of electron propagator theory, ionization potential equation-of-motion coupled cluster, and $\Delta$ -self-consistent field approaches in assigning photodetachment spectra	Abigail Gyamfi, Marco Caricato, Hrant Hratchian	Hall B2/C

## Tuesday, March 25

Time		Type	Title	Presenter & Co-Authors	Location
9:40 AM -	10:00 AM	Talk	Connecting strong and weak correlations with nonorthogonal configuration interaction	Chong Sun, Fei Gao, Gustavo Scuseria	Hall F Room 2
10:00 AM -	10:20 AM	Talk	Reducing the cost of TD-CI simulations of strong field ionization	H. Bernard Schlegel, Andrew Durden	Hall F Room 2
4:00 PM -	4:20 PM	Talk	Real-time simulations of preferential spin transport in chiral materials due to the chiral induced spin selectivity effect	<b>Xuechen Zheng,</b> Shiv Upadhyay, Tian Wang, Agam Shayit, Mengqi Yang, Xiaosong Li	Room 32B
7:00 PM -	9:00 PM	Poster	Silanol functionalization of amorphous silica surface	Shreyaa Brahmachari, Marco Caricato	Hall B2/C
7:00 PM -	9:00 PM	Poster	Improved methods for optimizing transition structures and Valley-Ridge inflection points	Cristian Sarabia, Ryan Baxter, Hrant Hratchian	Hall B2/C
7:00 PM -	9:00 PM	Poster	Prediction of polybasic macrocycles pKa: A black box computational workflow	<b>Tatum Harvey, Kristof Pota,</b> Magy Mekhail, David Freire, Benjamin Janesko, Kayla Green	Hall B2/C
7:00 PM -	9:00 PM	Poster	Comparison of DFT functionals and basis sets for geometry optimizations of cobalt complexes with ammonia, chloride, and water ligands	Simran Waraich, Sana Omar, Anna Lester, Peng Tao	Hall B2/C

## Sessions of Interest ( To Gaussian Users

#### Wednesday, March 26

Time Type	Title	Presenter & Co-Authors	Location
8:20 AM - 8:40 AM Talk	Generalized internal coordinates and intrinsic reaction coordinates used together	<b>Edward Brothers,</b> Alexander Marenich, Giovanni Scalmani, Michael Frisch	Hall F Room 2
10:20 AM - 10:40 AM Talk	Exploring thiol's surprising reactivity and selectivity over alcohol: A combined computational and experimental study on phenanthroline-catalyzed furanosylations	<b>Neha Rani,</b> Boddu S. Ramakrishna, H. Bernard Schlegel, Hien Nguyen	Hall F Room 2
11:40 AM - 12:00 PM Talk	Using constrained-self-consistent field and maximum overlap method schemes with spin- projection for computational studies of transition metal complexes	Brianna Aguilar-Solis, Aurora Pribram-Jones, Hrant Hratchian	Hall F Room 2
3:00 PM - 3:20 PM Talk	Isotope effect in optical rotation	Marco Caricato, Brian Faintich, Taylor Parsons, Ty Balduf	Hall F Room 2
3:40 PM - 4:00 PM Talk	Modeling photoelectron angular distributions for photodetachment spectra assignment using $\Delta\textsc{-SCF}$ Dyson orbitals	Andrew Bovill, Hrant Hratchian, Hassan Harb	Hall F Room 2
4:20 PM - 4:40 PM Talk	Simulating absorption spectra using EOM-CCSD with a polarizable force field: Application to the GFP chromophore	<b>Taylor Parsons,</b> Andrew Snider, Arthur Pyuskulyan, Christine Isborn, Marco Caricato	Hall F Room 2
4:40 PM - 5:00 PM Talk	Comparison of trajectory-based correlation function and Franck-Condon methods in optical spectroscopy: insights into spectral broadening and molecular interactions	Arthur Pyuskulyan, Christopher Myers, Christine Isborn	Hall F Room 2
5:00 PM - 5:20 PM Talk	Computing excitonic couplings of chromophores in solution	<b>Sayan Adhikari,</b> Ajay Khanna, Christopher Myers, Liang Shi, Christine Isborn	Hall F Room 2

#### Thursday, March 27

Time Typ	e Title	Presenter & Co-Authors	Location
8:00 AM - 8:20 AM Talk	Controlling rates and reversibilities of hydroxybenzylamine self-immolative linkers by tuning dearomatization energies	<b>Felix Fu,</b> Joseph Treacy, Brock Hosier, Kendall Houk, Heather Maynard	Room 30E



Highlighted Talk:

"Generalized internal coordinates and intrinsic reaction coordinates used together"

Presented by: Edward Brothers | Wednesday, March 26 | 8:20 AM - 8:40 AM | Hall F, Room 2