

# Division of Physical Chemistry

## Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Ernest N. Morial Convention Center: Room 225

H. Cuppen, D. E. Woon, *Organizers*

### SUNDAY AFTERNOON

#### Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Spectra & Properties

David. E. Woon, *Presiding*

**1:30** Introductory Remarks.

**1:35 : 86.** Accurate structure and spectroscopy of small molecular systems of astrophysical interest. T. Trabelsi, **J.S. Francisco**

**2:10: 87.** Quantum-chemical needs from the viewpoint of the Cologne Database for Molecular Spectroscopy. **H.S. Müller**

**2:45 : 88.** Spectroscopic characterization of key aromatic and heterocyclic molecules: A route toward the origin of life. **C. Puzzarini**, V. Barone, J. Bloino, N. Tasinato

**3:05** Intermission.

**3:25 : 89.** Answering unique spectroscopic and astrochemical problems through quantum chemistry. **R.C. Fortenberry**, K.A. Kloska, J.P. Layfield, C.M. Novak, T.J. Lee

**4:00: 90.** Exploring the rotational and far infrared spectra of non-rigid species using highly correlated ab initio methods. **M.S. Senent**

**4:35 : 91.** Infrared spectra of interstellar complex organic molecules: accurate energies and intensities by an anharmonic perturbative treatment. **J. Bloino**, A. Baiardi, C. Puzzarini, V. Barone

**4:55 : 92.** Chocolate molecules in space: Utilizing tunable vacuum ultraviolet light for isomer specific detection of complex organic molecules from astrophysical ice analogues. **M. Abplanalp**, S. Góbi, A. Bergantini, A.M. Turner, R. Kaiser

### MONDAY MORNING

#### Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Spectra & Properties/Gas-Phase Collisions

Ryan C. Fortenberry, *Presiding*

**8:30: 134.** Spectroscopic, theoretical, and observational study of aminomethanol, a predicted interstellar precursor to glycine. **S.L. Widicus Weaver**, B. Hays, M. McCabe, C. Powers, J. McMillan, S. Zinga

**9:05 : 135.** Probing magnetic fields with methanol masers and ro-vibrational collision rates for modeling protoplanetary disks. **G.C. Groenenboom**, B. Lankhaar, A. van der Avoird

**9:40: 136.** Exploration of the structure and spectrum of  $\text{CH}_5^+$  using diffusion Monte Carlo. **A.B. McCoy**, M.E. Fore

**10:00: 137.** Inorganic computational astrochemistry: Rovibrational quartic force fields. **N.J. Deyonker**, R.C. Fortenberry, Q. Cheng

**10:20: 138.** Diffuse interstellar bands and the pseudo-Jahn-Teller distortion in  $\text{C}_{60}^+$ . **S. Ahmadvand**, A.O. Lykhin, **S.A. Varganov**

**10:40** Intermission.

**11:00: 139.** Computing collisional energy exchange: Theory, old and new, and comparison with experiments. **L. Wiesenfeld**

**11:35 : 140.** Full-dimensional quantum dynamics of CO, CN, SiO, and CS in collisions with  $\text{H}_2$ . **B. Yang**, P. Zhang, C. Qu, P. Stancil, J.M. Bowman, B. Naduvalath, R. Forrey

**12:10: 141.** Mixed quantum/classical theory of molecular collisions: Applications to rotational-vibrational inelastic scattering in astrophysical environments. **D. Babikov**

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## MONDAY AFTERNOON

### Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Gas-Phase Reactions

Dahbia Talbi, *Presiding*

**1:30: 188.** High accuracy ab initio kinetics as a tool for astrochemistry. **S.J. Klippenstein**

**2:05 : 189.** Nonadiabatic dynamics in warm dense matter and small molecules. **A.V. Akimov**

**2:25 : 190.** State-of-the-art thermochemical and kinetic computations for complex organic molecules: Gas-phase formation routes in cold interstellar clouds. **V. Barone**, N. Tasinato, J. Bloino, D. Skouteris, C. Puzzarini

**2:45 : 191.** Kinetic measurements of  $\text{CO}^+$  and  $\text{CO}_2^+$  reactions with N and O atoms for models of planetary atmospheres and the interstellar medium. **J. Tenewitz**, T. Le, S.G. Ard, N. Shuman, A.A.

Viggiano, **J. Melko**

**3:05** Intermission.

**3:25 : 192.** Reaction mechanisms and rate constants of PAH growth in astrophysical environments.

**A.M. Mebel**

**4:00: 193.** Dynamics of pure and N-substituted cyclic aromatic hydrocarbon formation in the gas-phase. **P. Bera**, T. Stein, M.P. Head-Gordon, T.J. Lee

**4:35 : 194.** Modelling dehydrogenation in interstellar PAHs. **P. Castellanos**, **A. Candian**, H. Linnartz, X. Tielens

## TUESDAY MORNING

**Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Gas-Phase Reactions**

Stephen J. Klippenstein, *Presiding*

**8:30: 254.** Withdrawn

**9:05 : 255.** Nonadiabatic dynamics of silicon chemistry. **A.H. Chang**, R. Kaiser

**9:40: 256.** Reaction rates and mechanism for the reaction of electronically excited sulfur dioxide with alkanes. **J.A. Kroll**, V. Vaida

**10:00: 257.** Theoretical investigation of possible formation routes of interstellar SiS. **M. Rosi**, L. Mancini, N. Balucani, N. Faginas Lago, C. Ceccarelli, B. Le Floch, D. Skouteris, L. Podio, C. Codella, F. Fontani

**10:20** Intermission.

**10:40: 258.** How to obtain accurate diabatic surfaces governing the dissociative recombination of astrophysical ions. **D. Talbi**, D. Kashinski, P. Hickman

**11:15 : 259.** Computational study of the formation of prebiotic molecules in the interstellar medium through gas-phase reactions. **A. Largo**, P. Redondo, C. Barrientos, F. Siro Brigiano, Y. Jeanvoine, R. Spezia

**11:50: 260.** High accuracy thermochemistry and kinetics of the HCN/HNC system. **K. Lee**, M.C. McCarthy

## WEDNESDAY MORNING

**Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Surface Interactions/Grain Chemistry**

Thanja Lamberts, *Presiding*

**8:30: 308.** Off-lattice microscopic Monte Carlo kinetics models of interstellar and laboratory ices.

**R.T. Garrod**

**9:05 : 309.** A hybrid QM/MM approach to calculate binding energies of radical species on crystalline water ice . **W.C. Sameera**, B. Senevirathne, S. Andersson, G. Nyman

**9:40: 310.** Controversial determination of a key parameter to astrochemistry: Adsorption energy.

**F. Pauzat**

**10:00: 311.** Simulations of energy dissipation and non-thermal desorption on amorphous solid water. **A. Fredon**, H. Cuppen

**10:20** Intermission.

**10:40: 312.** Role of grain surfaces in astrochemical processes. **A. Rimola**, P. Ugliengo, C. Ceccarelli, **N. Balucani**, **M. Sodupe**

**11:15 : 313.** Experimental studies on the surface reaction of hydrogen sulfide with deuterium atoms on amorphous solid water at 10 K. **Y. Oba**

**11:50: 314.** Reaction experiments on H exposure of solid methanol at low temperatures. **Y. Yarnall**, H. Hidaka, Y. Oba, T. Hama, A. Kouchi, N. Watanabe

## WEDNESDAY AFTERNOON

**Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Grain Chemistry / Modeling: Protostellar Disks**

Robin T. Garrod, *Presiding*

**1:30: 359.** Reactivity of atoms and molecules on interstellar ice analogs at low temperatures. **T. Lamberts**, J. Kästner

**2:05 : 360.** Methanol-containing ice mantle on collision with OH: A dust grain reaction through quantum *ab initio* molecular dynamic. **N. Inostroza**

**2:40: 361.** Mechanisms of SiO oxidation: Implications for dust formation. **S. Andersson**

**3:00: 362.** Trapping of molecular oxygen in cometary ices: solid state modeling. **A. Markovits**

**3:20** Intermission.

**3:40: 363.** New constraints on the chemistry of planet formation. **E. Bergin**

**4:15 : 364.** Gaining insights into protoplanetary disk conditions from chemistry. **U. Gorti**

## THURSDAY MORNING

**Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments: Modeling: ISM/Clouds & (Exo)Planetary Atmospheres**

H. Cuppen, *Presiding*

**8:30: 626.** Help is needed: Some current astrochemical problems. **E. Herbst**

**9:05 : 627.** Astrochemical kinetic models of dark molecular clouds: Statistical methods and TMC-1.

**D. Maffucci**, E. Herbst

**9:25 : 628.** Deuterium fractionation from molecular clouds to protoplanetary disks: Modeling and observation. **L. Majumdar**

**9:45 : 629.** The unusual dynamics and chemistry in planetary nebulae. **L.M. Ziurys**, D. Schmidt, L.N. Zack, N. Woolf

**10:05 : 630.** Modeling the chemistry in the complex outflows of supergiant stars. **D. Schmidt**, G. Adande, L.M. Ziurys

**10:25** Intermission.

**10:45 : 631.** Atmospheric chemistry on Venus: An overview of unresolved issues. **F. Mills**, E. Marcq, Y. Yung, C. Parkinson, K. Jessup, A. Vandaele

**11:20: 632.** Modeling exoplanet atmospheric chemistry in the era of the James Webb Space Telescope. **S. Horst**

**11:55 : 633.** From the rocky kernel to the exosphere: the journey of alkali in Europa. **Y. Ellinger**