Program STC 2015

Sunday, September 20th		
14:00 – 17:00		**Arrival and Registration**
17:00 – 17:15	P. Saalfrank	**Opening**
Session 1: Opening Session (Chair: G. Frenking)		
17:15 – 18:15	**I1:** B. Friedrich	*How did the tree of knowledge get its blossom? The rise of physical and theoretical chemistry*
18:15 – 18:35	**C1:** C. König	*Generation and exploitation of locality in vibrational calculations*
18:35 – 18:55	**C2:** L. v. Szentpaly	*Thermocyclic equations and symmetry laws to explain and limit conceptual DFT principles*
19:00 – 21:00		**Welcome reception**

Monday, September 21st		
Session 2: Electron dynamics (Chair: H.P. Lüthi)		
09:00 – 09:45	**I2:** L. Cederbaum	*On systems with and without excess energy in environment ICD and other interatomic mechanisms*
09:45 – 10:05	**C3:** A. Bande	*Phonon impact on energy transfer processes in double quantum dots*
10:05 – 10:25	**C4:** A. Schild	*Exact electron factorization perspective on high harmonic generation*
10:30 – 11:00		**Coffee break**
Session 3: Reaction dynamics (Chair: B. Hartke)		
11:00 – 11:45	**I3:** S. Althorpe	*Is there a quantum transition-state theory?*
11:45 – 12:05	**C5:** I. Ulusoy	*Reconciling roaming reaction pathways and transition state theory*
12:05 – 12:25	**C6:** J. O. Richardson	*Non-adiabatic ring-polymer molecular dynamics: Electron-transfer rates and vibronic spectra*
12:30 – 14:00		**Lunch**
Session 4: First-Principles MD (Chair: D. Marx)		
14:00 – 14:45	**I4:** B. Kirchner	*Complex molecular and ionic liquids from first-principles molecular dynamics simulations*
14:45 – 15:05	**C7:** D. Muñoz-Santiburcio	*Reactive dynamics in nanoconfined water: Implications for prebiotic chemistry*
15:05 – 15:25	**C8:** S. Luber	*Computationally efficient approaches for liquids and homogeneous catalysis*
15:30 – 16:00		**Coffee break**
Session 5: Excited Sates I (Chair: W. Thiel)		
16:00 – 16:45	**I5:** L. González	*Excited states for complex systems: Phase-space sampling and environment*
16:45 – 17:05	**C9:** D. Tuna	*Excited states, conical intersections, and photochemistry of (bio-)organic molecules*
17:05 – 17:25	**C10:** J. Tatchen	*Computation of vibronic spectra by a combination of frozen gaussian semiclassical dynamics and potential energy surface interpolation*
17:30 – 17:45		**Presentation SCM**
17:45 – 18:45	C. Ochsenfeld	**Meeting AGTC**
19:00 – 20:00		**Dinner**
20:00 – 22:00		**Poster Session I (odd numbers)**

Tuesday, September 22nd		
Session 6: DFT I (Chair: W. Klopper)		
09:00 – 09:45	**I6:** A. Görling	*Density-functional methods based on the adiabatic-connection fluctuation-dissipation theorem combining high accuracy and wide applicability*
09:45 – 10:05	**C11:** H. Bahmann	*Local hybrid density functionals from an interpolation of the adiabatic connection between the exchange and the strong-correlation limit*
10:05 – 10:25	**C12:** J. Friedrich	*Binding energies of large clusters: DFT is better than expected!*
10:30 – 11:00		**Coffee break**

Session 7: DFT II (Chair: A. Dreuw)		
11:00 – 11:45	**I7:** M. Head-Gordon	*Survival of the most transferable: New semi-empirical density functionals from a combinatorial design strategy*
11:45 – 12:05	**C13:** A. D. Boese	*Hydrogen bonds: The accuracy of post-Hartree-Fock and density functional methods*
12:05 – 12:25	**C14:** V. Krewald	*Prediction of redox potentials for magnetically coupled transition metal clusters*
12:30 – 14:00		**Lunch**
Session 8: Solids (Chair: B. Paulus)		
14:00 – 14:45	**I8:** A. Alavi	*Full CI quantum Monte Carlo: Method and recent developments*
14:45 – 15:05	**C15:** D. Usvyat	*Approaching sub-kJ/mol accuracy in solid state applications by combined periodic/ finite-cluster quantum chemical treatment*
15:05 – 15:25	**C16:** R. Tonner	*Explaining unusual reactivity in extended systems with energy-based analyses*
15:30 – 16:00		**Coffee break**
Session 9: Surfaces (Chair: A. Groß)		
16:00 – 16:45	**I9:** T. Seideman	*Current-driven phenomena in junctions. An ensemble scattering theory applied to three bizarre reactions*
16:45 – 17:05	**C17:** G. Füchsel	*Reactive scattering of CD_3H on Pt(111): A quantum dynamical description*
17:05 – 17:25	**C18:** A. Kandratsenka	*NO vibrational energy transfer on Au(111) surface: A challenge to the first-principles theory*
17:25 – 17:45	**C19:** J. Paier	*Hydration of the Fe_3O_4(111) surface: When static calculations anticipate a dynamic scenario*
18:00 – 19:00		**Dinner**
19:00 – 22:00		**Poster Session II (even numbers)**

Wednesday, September 23rd		
Session 10: DFT III (Chair: Ch. Marian)		
09:00 – 09:45	**I10:** S. Grimme	*Simple quantum chemistry for comples systems and processes*
09:45 – 10:05	**C20:** I. Lyskov	*Redesigned DFT/MRCI*
10:05 – 10:25	**C21:** M. Korth	*Computational screening of battery electrolyte materials*
10:30 – 11:00		**Coffee break**
Session 11: Electronic Structure (Chair: T. Körzdörfer)		
11:00 – 11:45	**I11:** R. Baer	*Charge-carrier localization in extended systems*
11:45 – 12:05	**C22:** P. A. Limacher	*Seniority-zero wavefunctions: How to treat multi-reference problems with single-reference ansätze*
12:05 – 12:25	**C23:** J. Kussmann	*Low-scaling quantum chemical methods on massively parallel architectures: What's to learn from GPUs?*
12:30 – 14:00		**Lunch**
14:00 – 18:00		**Excursions / Free afternoon**
19:00 – 22:00		**Conference dinner**

Thursday, September 24th		
Session 12: Materials (Chair: Ch. v. Wüllen)		
09:00 – 09:45	**I12:** C. Draxl	*Theoretical spectroscopy of π-conjugated molecules and their condensed phases*
09:45 – 10:05	**C24:** A. Prlj	*Excited states conundrum and nonadiabatic molecular dynamics of thiophene-based compounds*
10:05 – 10:25	**C25:** J. Megow	*Calculating optical spectra of supramolecular aggregates demands treatment of site-dependent dispersive excitation energy shifts*
10:30 – 11:00		**Coffee break**
Session 13: Excited States II (Chair: R. Berger)		
11:00 – 11:45	**I13:** R. Mitrić	*Light-induced nonadiabatic dynamics in molecules and nanostructures*
11:45 – 12:05	**C26:** E. Hedegård	*Treating solutes and protein chromophores properly: Polarizable embedding with correlated wave functions*
12:05 – 12:25	**C27:** E. Gindensperger	*Spin-vibronic excited-state quantum dynamics in transition metal complexes*
12:30 – 13:00	P. Saalfrank, T. Klamroth	**Poster prizes / closing**
13:00 –		**Lunch, departure**