Telluride workshop schedule: From ab initio Computations to Conceptual Insights into Bonding

Workshop location: Telluride Innovation Center, 300 S Townsend St., Telluride, CO 81435

Monday 05/26

5:00pm-6:30pm : Cash bar meet and greet at Alibi 157 S. Fir Street

Tuesday 05/27

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| 12:25 -1:00 | Vanda Glezakou | | |  |
| 1:00-1:35 | Ping Yang | | |  |
| 1:35 – 2:10 | Beltran Leiva, Maria | | |  |
| 2:10 – 2:45 | Henk Eshuis *The impact of heteroatoms on the aggregation of asphaltene model systems*. | | |  |
| 2:45 –3:00 |  | | **coffee break** | |
| 3:00 –3:35 | Ken Jordan *On the Role of Charge-flow in the Polarizability and Polarization Potentials of Polyaromatic Hydrocarbons of Increasing Size and Extrapolation to the Image Potential of Graphene* | | |  |
| 3:35 –4:10 |  | John Keith *Post-semiempirical quantum mechanics methods* | | |
| 4:10 –4:45 | Jane Murray *A Look at Bonds and Bonding* | | |  |

Wednesday 05/28

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| 8:25-9:00 | Sason Shaik *A Gravitational-Like Relationship of Dispersion Interactions is Exhibited by 40 Pairs of Molecules and Noble Gas Atoms* |  |
| 9:00 – 9:35 | Klaus Ruedenberg *Atoms and bonds as synergisms of interactions between electrons and nuclei inherent in molecular electronic wave functions* |  |
| 9:35-10:10 | Daniel Del Angel Cruz *A wave function-intrinsic energy decomposition analysis for polyatomic molecules* |  |
| 10:10 -10:25 | **Coffee break** |  |
| 10:25-11:00 | Mark Gordon |  |
| 11:00-11:35 | George Schoendorff *Chemical Bonding in the f-Block* |  |
| 11:35-12:10 | Juan Duchimaza *Characterization of Bonding Patterns by ab initio Quasi-Atomic Orbital Analyses* |  |
| 5:30-7:00 | Picnic |  |

Thursday 05/29

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| 8:25-9:00 | Emilie Guidez *Quasi-atomic orbital analysis of sigma-hole interactions* |  |
| 9:00 – 9:35 | Sotiris Xantheas: *Pairwise additive and many-body non-additive effects in chalcogen bonds juxtaposed to the ones in hydrogen bonds* |  |
| 9:35 – 10:10 | |  | | --- | | Martin Head-Gordon *Beyond numerical experiments: Understanding physical and chemical driving forces by energy decomposition analysis* | |  |
| 10:10-10:25 |  | **coffee break** |
| 10:25 -11:00 | Martin Rahm |  |
| 11:00-11:35 | David Sherrill *Insights into substituent effects in protein-ligand interactions through symmetry-adapted perturbation theory* |  |
| 11:35-12:10 | Gernot Frenking *The description of unusual bonds in molecules with quantum chemical methods* |  |

Friday 05/30

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| 8:25-9:00 | Marco A C Nascimento *THE INTERFERENCE ENERGY ANALYSIS OF UNSUAL (?) CHEMICAL BONDS AND OF ENERGY BARRIERS FOR CHEMICAL REACTIONS.* |  |
| 9:00 – 9:35 | Philippe Hiberty *Valence Bond alternative yielding insightful and accurate wave functions for challenging excited states. Application to ethylene, ozone and sulfur dioxide.* |  |
| 9:35 – 10:10 | Thom Dunning *Beyond MO and VB Theories:*  *Spin-Coupled Generalized Valence Bond Theory of the Electronic Structure of Molecules* |  |
| 10:10 –10:25 | **coffee break** |  |
| 10:25 –11:00 | Tore Brinck*.* |  |
| 11:00 –11:35 | Tosaporn Sattasathuchana |  |
| 11:35-12:10 | Joe Ivanic |  |