

# Program

Monday, 04.11.2013

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|--|---------------------------|--|
| Morning  |                           | Arrival and Registration   |
| 13:50 – 14:00  | Saalfrank                 | Welcome  |
| <b>Session 1: Atom scattering: From diffraction to atom optics (I)</b> |                           |  |
| <i>Chair: P. Saalfrank</i>   |                           |  |
| 14:00 – 14:40  | I1: Toennies              | The interaction of hard helium atoms with soft electrons at metal surfaces           |
| 14:40 – 15:20  | I2: Pollak                | Quantum diffraction and coherence of heavy particles scattered from surfaces         |
| 15:20 – 16:00  | I3: Ernst                 | Vibrational dynamics and surface structure of semimetals from helium atom scattering |
| 16:00 – 16:30  |                           | Coffee Break   |
| <i>Chair: M. Nest</i>  |                           |  |
| 16:30 – 17:10  | I4: Winter                | Fast Atom Diffraction (FAD)  |
| 17:10 – 17:50  | I5: Hornberger            | Grating interaction effects in molecular near-field interferometry                   |
| 17:50 – 18:10  | C1: Eder,<br>Kaltenbacher | NEMI – NEutral (Helium) MIcroscopy   |
| 18:10 – 18:30  | C2: Witham                | Neutral atom microscopy: recent results and prospects                                |
| 18:30 – 20:00  |                           | Dinner   |

**Tuesday, 05.11.2013**

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|---|-----------------|---|
| <b>Session 2: Hydrogen and hydrogen scattering (I)</b>    |                 |   |
| <i>Chair: A.W. Kleyn</i>                                  |                 |   |
| 09:00 – 09:40   | I6: Kroes       | Towards a chemically accurate description of reactive molecule-surface scattering   |
| 09:40 – 10:20   | I7: Farías      | Molecular beam studies of dissociation of H <sub>2</sub> and O <sub>2</sub> on bimetallic surfaces  |
| 10:20 – 10:40   | C3: Díaz        | Diffraction of H from LiF(100) under fast grazing incidence conditions: the role of the structure factor  |
| 10:40 – 11:10   | Coffee Break    |   |
| <i>Chair: R. Beck</i>                                     |                 |   |
| 11:10 – 11:50   | I8: Hasselbrink | Hydrogenation of epitaxial graphene: from graphene to graphane  |
| 11:50 – 12:30   | I9: Martinazzo  | Hydrogen atoms on graphene: structure, energetics and dynamics  |
| 12:30 – 14:00   | Lunch           |   |
| <b>Session 3: Complex scatterers and complex surfaces</b> |                 |   |
| <i>Chair: A.M. Wodtke</i>                                 |                 |   |
| 14:00 – 14:40   | I10: Kleyn      | Eley-Rideal reactions with hyperthermal N atoms   |
| 14:40 – 15:20   | I11: Díez Muiño | Nitrogen atoms and molecules landing, reacting, and rebounding at metal surfaces  |
| 15:20 – 16:00   | I12: Beck       | State-resolved gas/surface reactivity: probing the role of vibration in dissociative chemisorption  |
| 16:00 – 16:30   | Coffee Break    |   |
| <i>Chair: J. Tully</i>                                    |                 |   |
| 16:30 – 17:10   | I13: Jackson    | The dynamics of the dissociative chemisorption of methane on Ni and Pt surfaces: the effects of substrate temperature and molecular vibrational state |
| 17:10 – 17:50   | I14: Sibener    | Dynamical processes of gas-surface encounters at ice and organic interfaces   |
| 17:50 – 18:10   | C4: Busnengo    | Molecular dynamics study of methane dissociation on Ni(111) and Pt(111)   |
| 18:10 – 18:30   | C5: Smerieri    | In-situ combination of supersonic molecular beam and low temperature STM  |
| 18:30 – 20:00   | Dinner          |   |
| 20:00 – 22:00   | Poster Session  |   |

**Wednesday, 06.11.2013**

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| <b>Session 4: Non-adiabatic processes and photochemistry</b> |                   |  |
| <i>Chair: E. Hasselbrink</i>                                 |                   |  |
| 09:00 – 09:40  | I15: Wodtke       | New perspectives in dynamics at surfaces   |
| 09:40 – 10:20  | I16: Tully        | Quantum-classical strategies for dynamics at surfaces  |
| 10:20 – 10:40  | C6: Kandratsenka  | H-atom scattering from Au(111): classical MD on a full-dimensional EMT potential energy surface                    |
| 10:40 – 11:10  |                   | Coffee Break   |
| 11:10 – 11:50  | I17: Kosloff      | Hot injection processes in optically-excited states: molecular design for optimized photocapture                   |
| 11:50 – 12:30  | I18: Klüner       | A first principles approach to photochemistry at surfaces  |
| 12:30 – 13:30  |                   | Lunch  |
| <i>Chair: T. Klamroth</i>                                    |                   |  |
| 13:30 – 14:10  | I19: Arnolds      | Inducing non-adiabatic effects through coadsorption: energy transfer between CO and Cu(110) mediated by porphyrins |
| 14:10 – 14:30  | C7: Meyer         | Non-adiabatic vibrational damping of O <sub>2</sub> on Ag(100): implications for light-enhanced catalysis?         |
| 14:30 – 14:50  | C8: Diño, Shimizu | Dynamics of O <sub>2</sub> dissociative adsorption and abstraction on Al(111)                                      |
| 15:30 – 19:00  |                   | Conference Outing  |
| 19:00 – 22:00  |                   | Dinner   |

Thursday, 07.11.2013

**Session 5: Hydrogen and hydrogen scattering (II)**

*Chair: G.-J. Kroes*

|               |                  |  |
|---------------|------------------|--|
| 09:00 – 09:40 | I20: Juurlink    | H <sub>2</sub> , O <sub>2</sub> and H <sub>2</sub> O on nanostructured surfaces                                    |
| 09:40 – 10:00 | C9: Füchsel      | The role of electronic friction for scattering and dissociative adsorption of H <sub>2</sub> molecules on Ru(0001) |
| 10:00 – 10:20 | C10: Schauermann | Hydrogen on supported Pd nanoparticles: adsorption and reactivity  |
| 10:00 – 10:20 | C11: Bünermann   | Inelastic hydrogen atom scattering: a new tool to investigate energy conversion processes at surfaces              |
| 10:40 – 11:10 |                  | Coffee Break   |

**Session 6: Atom scattering: From diffraction to atom optics (II)**

*Chair: E. Pollak*

|               |                  |  |
|---------------|------------------|--|
| 11:10 – 11:50 | I21: Miret-Artés | Bohmian mechanics: from atom optics to surface scattering        |
| 11:50 – 12:30 | I22: Allison     | Quantum effects in the motion of atoms and molecules at surfaces |
| 12:30 – 12:40 |                  | Closing Remarks  |
| 12:40 – 14:00 |                  | Lunch and Departure  |