# Program

## Sunday, August 24<sup>th</sup>

16.30–18.30 Registration
17.30–18.30 Reception
18.40–18.50 Welcome – Gunnar Nyman
18.50–19.00 Welcome – Dean of Science, Elisabet Ahlberg

Chair: Dag Hanstorp

19.00–20.00 I1: Richard Zare, Preparation of Molecular Hydrogen in a Controlled Superposition of  $|vJM\rangle$  States

 $20.00-21.00 \text{ I2: David Manolopoulos, Photochemistry, semiclassical spin dynamics, and the avian navigation problem$ 

# Monday, August 25<sup>th</sup>

Theory, Chair: Sture Nordholm

09.00 I3: Uwe Manthe, State-resolved quantum dynamics of polyatomic reactions 09.40 I4: Irene Burghardt, Quantum dynamics of exciton migration and dissociation in functional organic polymer materials 10.20 C1: Rita Prosmiti, The role of large-amplitude motions in the IR spectra of  $H_5^+/D_5^+$  cations 10.40 Coffee

11.10 I5: Stuart C. Althorpe, Is there a quantum transition-state theory?

11.50 I6: Nandini Ananth, Novel Path-Integral Based Dynamics for Photochemistry

12.20 C2: Jeremy O. Richardson, Nonadiabatic ring-polymer molecular dynamics rate theory

## 12.40-14.00 Lunch

Experiments, Chair: Mats Larsson

14.00 I7: Kopin Liu, Effects of reagent rotational excitation on Cl + CH<sub>4</sub>/CHD<sub>3</sub> reactions
14.40 I8: Ian Sims, Radical reactivity at very low temperatures
15.10 C3: Astrid Bergeat, Crossed-beam inelastic scattering experiments at energies approaching the cold regime
15.30 Coffee
16.00 I9: Gerard Meijer, Taming beams of neutral molecules
16.40 I10: Mark Brouard, The stereodynamics of inelastic scattering of NO(X) by the rare gases

17.20 C4: Matthew Costen, Probing the surface of ionic liquids through collisions with gas-phase atoms 17.40 C5: Thomas Pino, Intramolecular processes revealed using UV-Laser-Induced IR-Fluorescence of the first electronic transition of Benzene

# Monday evening – City of Gothenburg reception 19.00–20.30

#### Tuesday, August 26<sup>th</sup>

Astrochemistry/astrophysics, Chair: Stefan Andersson

09.00 I11: Eric Herbst, Gas-Grain Chemical Simulations of Star-forming Regions 09.40 I12: Liv Hornekær, Polycyclic aromatic hydrocarbons as catalysts for interstellar chemical complexity 10.10 C6: Victor Herrero, Vibrational spectroscopy and kinetics of the astronomically relevant  $ArH^+$  ion in  $Ar/H_2$  cold plasmas

10.30 Coffee

11.00 I13: Laurent Wiesenfeld, Molecular collisions for Astrophysics: theory and experiments 11.40 I14: Herma Cuppen, Kinetic Monte Carlo simulations of interstellar grain surface chemistry 12.10 C7: Nathalie de Ruette, Merged beam studies for astrobiology

12.30-14.00 Lunch

Theory, Chair: Magnus Gustafsson

14.00 I15: Donghui Zhang, Differential Cross Sections for the H+CD<sub>4</sub> and H+SiH<sub>4</sub> reactions
14.40 I16: Octavio Roncero, State-to-state reactive collisions with H<sub>2</sub> of astrophysical interest
15.10 C8: Judith Rommel, Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling
15.30 Coffee
16.00 I17: Tamar Seideman, Control of Transport and Mechanical Motions in Junctions with Coherent light
16.40 I18: Terry Frankcombe, New Gaussian basis set methods for quantum systems
17.10 I19: Anthony Meijer, Quantum dynamics studies of surface-catalysed H atom recombination
17.40 C9: Jens Poulsen, The Classical Wigner model and the ensemble conserving problem
18.15–19.30 Dinner
19.30–21.30 Poster session (odd numbered posters)

## Wednessday, August $27^{\text{th}}$

Experiments, Chair: Raimund Feifel

09.00 I20: Murthy Gudipati, Chemical Reaction Dynamics in Cryogenic Ices in Our Galaxy 09.40 I21: Henrik Cederquist, Fragmentation of polycyclic aromatic hydrocarbons and their clusters and ion storage in DESIREE

10.10 C10: Alexandre Perret, Temperature dependence of dissolved  $CO_2$  diffusion in Champagne wines: a theoretical and experimental investigation

 $10.30~{\rm Coffee}$ 

11.00 I22: Lars H. Andersen, Time-resolved action spectroscopy in ion storage rings

11.40 I23: Vitali Zhaunerchyk, Site-specific fragmentation of varying size molecules induced by resonant K-shell excitation

12.10 C11: David Bonhommeau, Structure and stability of multiply-charged clusters: Application to charged droplets produced by electrospray ionisation

#### Wednesday afternoon – boat excursion with lunch 13.30–16.30

17.00–19.00 Poster session (even numbered posters)

## Thursday, August 28<sup>th</sup>

Atmospheric chemistry, Chair: Matthew Johnson

09.00 I24: Kristie A. Boering, Reaction dynamics and kinetics of oxygen isotope exchange reactions: Insights into unusual isotope effects and their applications in earth and planetary science

09.40 I25: Johan A. Schmidt, On the origin of the high levels of Br radicals in tropical free troposphere 10.10 I26: Theo Kurtén, Exploring atmospheric autoxidation using quantum chemistry 10.40 Coffee

11.10 C12: Ad van der Avoird, In depth experimental and theoretical studies of molecular collisions 11.30 C13: Morgane Vacher, Coupled electron-nuclear dynamics following photoionisation of benzenes 11.50 C14: Luís Viegas, Exploring the influence of water in ozone depletion through the  $HO_2 + nH_2O + O_3$ reaction: from a single water molecule to a water cage

12.10 C15: Gábor Czakó, Dynamics of polyatomic chemical reactions on ab initio potential energy surfaces

#### 12.30–14.00 Lunch

Control/Cold, Chair: Jens Poulsen

14.00 I27: Dmitry Shalashilin, Multidimensional quantum mechanics with trajectory guided basis sets of Coherent States. From nonadiabatic photochemical reactions to dynamics of electrons in strong laser field. 14.40 I28: Åsa Larson, Molecular dynamics involving electronic resonant states of HeH

15.10 C16: Adam Kirrander, *Theory and simulations for ultrafast x-ray scattering* 15.30 Coffee

16.00 I29: Olivier Dulieu, Radiative formation of cold molecular ions in an ion/atom hybrid trap 16.30 I30: Andreas Osterwalder, Penning Ionization Reactions of Polyatomic Molecules at Low Temperature 17.00 C17: Alberto García-Vela, Resonant detection of the signature of control on a resonance state lifetime using a pumpprobe scheme18.00 Theater play: Lise Meitner19.30 Conference dinner

Friday, August  $28^{th}$  – departure