Program

- Monday morning, June 26: **Fundamentals of intermolecular interactions:**
  Chair: Bogumil Jeziorski
  - 9:00–9:45 am William H. Adams, Department of Chemistry, Rutgers University
    Understanding Intermolecular Perturbation Theory
  - 9:55–10:40 am Konrad Patkowski, University of Delaware
    Ultra-SAPT: recent extensions of symmetry-adapted perturbation theory
  - 10:50–11:35 am Piotr Żuchowski, Faculty of Chemistry, University of Warsaw
    Recent advances in perturbation theory of intermolecular forces for van der Waals complexes containing open-shell monomers
  - 11:45–12:00 am Break
- Monday afternoon and evening: **Nonreactive dynamics of van der Waals clusters:**
  Chair: Ad van der Avoird
  - 12:00–12:45 pm Claude Leforestier, Université de Montpellier (France)
    A water dimer flexible potential from theoretical and experimental results
  - 7:00–7:45 pm Robert Hinde, University of Tennessee
    Vibrational dynamics in H_2 aggregates: from the van der Waals dimer to solid parahydrogen
  - 7:55–8:35 pm Richard Wheatley, University of Nottingham
    Van der Waals complexes of water and other atmospheric gases
- Tuesday morning, June 27: **Interactions involving open-shell systems:**
  Chair: Millard Alexander
  - 8:00–8:45 am Grzegorz Chałasiński
    Faculty of Chemistry, University of Warsaw, Poland
    Paradigm pre-reactive van der Waals complexes between open-shell atom and closed-shell molecule
  - 8:55–9:40 am Małgorzata M. Szczesniak, Department of Chemistry, Oakland University
    Interactions between d- and f-electron atoms and rare-gases
  - 9:50–10:20 am Łukasz Rajchel
    Faculty of Chemistry, University of Warsaw and Department of Chemistry, Oakland University
    Interaction between two transition metal atoms
  - 10:30–11:15 pm Ramon Hernandez-Lamoneda
    Centro de Investigaciones Quimicas, UAEMor, Cuernavaca, Mexico
    Intermolecular potentials and energy transfer processes in the O_2 + O_2 system

- Tuesday afternoon and evening **Cold collisions and very long-range interactions:**
  Chair: Robert Moszyński
  - 1:30–2:15 pm Bogumił Jeziorski, Faculty of Chemistry, University of Warsaw
    Theoretical determination of the scattering length of spin-polarized helium
  - 2:25–3:10 pm Roman Krems, University of British Columbia, Vancouver, Canada
    Collisions of atoms and molecules in electric and magnetic fields
  - 3:20–4:05 pm Gerrit C. Groenenboom, Radboud University Nijmegen, The Netherlands
    Stark controlled Xenon-OH collisions; potentials and dynamics
  - **6:00–7:15 pm** **Town Talk**: Millard H. Alexander
    Serendipity in physical chemistry: How discoveries are made
    Mountain Village Conference Center
  - 8:00–8:45 pm Balakrishnan Naduvalath, Department of Chemistry, University of Nevada Las Vegas
    Dynamics of Chemical Reactions at Cold and Ultracold Temperatures

- Wednesday morning and evening. June 28: **Interactions involving excited monomers and dynamics on multiple potential energy surfaces:**
  Chair: Claude Leforestier
  - 8:00–8:45 am Robert Moszyński, Faculty of Chemistry, University of Warsaw
    Long-range relativistic interactions in the excited states and quantum dynamics on coupled manifolds of potentials
  - 8:55–9:40 am Millard Alexander, Department of Chemistry, University of Maryland
    Treating open-shell atoms in quantum molecular dynamics simulations
  - 9:50–10:05 am Break
  - 10:05–10:50 am Marc van Hemert, Leiden University
    The excited water dimer
  - 11:00–11:45 am Ad van der Avoird, Radboud University Nijmegen, The Netherlands
    Properties and spectra of open-shell reaction precursor complexes: a multiple potential problem
  - 11:55–12:40 pm Octavio Roncero, Institut Matematicas y Fisica Fundamental, CSIC, Madrid (Spain)
    Coupled diabatic energy surfaces to study reaction dynamics at conical intersections: application to the photodetachment of OHF^-
  - 8:00–8:45 pm Jacek Kłos, Department of Chemistry, University of Maryland
    Quantum statistical studies of kinetics of the radical-radical reaction: $OH(v=0,1)+O \rightarrow O_2 + H$

- Thursday morning, June 29: **Applications of DFT in theory of intermolecular interactions:** Chair: Anthony Stone
  - 8:00–8:45 am Xi Chu, University of Montana
    A time-dependent density functional approach for dispersion interactions
  - 8:55–9:40 am David Langreth, Rutgers University
    Applications of van der Waals density functional (vdW-DF)
  - 9:50–10:05 am Break
  - 10:05-10:50 am Georg Jansen, Department of Chemistry, University Duisburg-Essen
    Density-fitting DFT-SAPT: Foundations and applications to CH-π and π-π interactions
  - 11:00–11:45 am Krzysztof Szalewicz, University of Delaware
    Symmetry-adapted perturbation theory with Kohn-Sham monomers: new developments and applications to large molecules
- Friday morning, June 30: **Towards systems containing dozens of atoms:** Chair: Krzysztof Szalewicz
  - 8:00–8:45 am Alexander Boldyrev, Utah State University, Logan
    Why Do All-Boron Clusters Prefer Planar or Quasi-planar Structure?
  - 8:55–9:40 am Vladimir Spirko, Prague
    Quasiplanarity of the Peptide Bond
  - 9:50–10:35 am P. Tarakeshwar, School of Computational Sciences, Korea Institute for Advanced Study, Seoul
    Characterization of Intermolecular Interactions Involving π Systems
  - 10:45–11:00 am Break
  - 11:00–11:45 am Anatoliy V. Volkov, SUNY at Buffalo
    Intermolecular atom-atom potentials for H, C, N and O atoms from Symmetry-Adapted Perturbation Theory
  - 11:50–12:35 pm Anthony Stone, University Chemical Laboratory, Cambridge University
    Derivation of atom-atom interaction potentials from Coupled Kohn-Sham calculations