SYQM 1: Precise Quantum Molecules

Time: Thursday 10:45–12:45 Location: ZHG105

Invited Talk SYQM 1.1 Thu 10:45 ZHG105

The quantum world of molecules revealed with rotational coherence spectroscopy — •Melanie Schnell — Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Early application of quantum modelling to molecules was limited to diatomics, mostly simple hydrogen. Experimental spectroscopy met such modelling with high precision. The recent developments of various types of experimental spectroscopies at an increasing level of sophistication allowed for their application to larger molecules and at an increasing level of complexity, including highly coherent quantum tunnelling and chirality studies. This lecture will provide some glimpses on the impressive history of spectroscopic experiments using the example of rotational excitations, from the MASER to modern control experiments.

Invited Talk SYQM 1.2 Thu 11:15 ZHG105

Accurate calculation of non-covalent interactions using explicitly correlated local correlation methods — •Hans-Joachim Werner[1], Andreas Hansen[2], and Peter J. Knowles[3] — [1]Institut für Theoretische Chemie, Universität Stuttgart, Germany — [2]Mulliken Center for Theoretical Chemistry, Universität Bonn, Germany — [3]School of Chemistry, Cardiff University, Cardiff CF10 3AT, U.K.

Recent developments of highly accurate electron correlation methods applicable to large molecular systems are reviewed. This includes local correlation approximations, explicit correlation methods, as well as fragmentation or embedding approximations. Using a combination of these approaches it has become possible to predict reaction energies, isomerization energies, conformational energies, and intermolecular interaction energies for systems with over hundred atoms with subkcal/mol accuracy. In this talk we present recent benchmark calculations [1] for non-covalent interactions (NCI) in large π-stacked molecular aggregates and host-guest systems using the PNO-LCCSD(T)-F12 method as implemented in Molpro. Key NCI systems previously evaluated using FN-DMC and other LCCSD(T) methods are reexamined with focus on the question whether CCSD(T) overbinds in large π-stacked complexes or other systems with high polarizability.

[1] A. Hansen, P. J. Knowles, and H.-J. Werner, J. Phys. Chem. A (2025), https://doi.org/10.1021/acs.jpca.5c02316

Invited Talk SYQM 1.3 Thu 11:45 ZHG105

High-resolution spectroscopy of molecular ions — •Stephan Schlemmer — I. Physikalisches Institut, Universität zu Köln

Spectroscopy is one of the foundations of quantum mechanics. For molecules the spectra usually break-up into the electronic, vibrational and rotational energy regime based on the Born-Oppenheimer approximation which separates the dynamics of the electrons from those of the nuclei. Vibrational spectra reveal the forces between the atoms constituing the molecule and rotational spectra are related to their mass distribution, i.e., the structure of the molecule and highly precise distances of the atomic nuclei. These findings lead to our today's picture of a molecule as a set of atoms (balls) bound by their electrons (sticks), where, e.g., the methane molecule, CH_4, has a pyramidal structure of the hydrogens with the carbon atom in the center entertaining one bond to each of the hydrogens. As a result of this success story of quantum mechanics complex molecules are found in space based on their fingerprint like spectra. I will present example spectra for molecular ions which have been discovered recently and which play an important role in interstellar chemistry. However, several well bond molecules are very floppy, meaning the nuclei undergo large amplitude motions and the picture of a molecular structure described above is called in question. Finding a proper quantum mechanical description for such systems as well as measuring their spectra is still a challenge today as will be discussed in this work.

Invited Talk SYQM 1.4 Thu 12:15 ZHG105

Quantum Simulations in the Chemical Industry — •Ansgar Schäfer — BASF SE, Carl-Bosch-Straße 38, 67056 Ludwigshafen, Germany

Chemical product and process development can be a challenging endeavor if the chemical and structural search space is huge, the number of tunable parameters is big, knowledge about mechanisms is sparse, and experiments are difficult to perform and/or expensive. Therefore, instead of relying on the conventional approach of trial-and-error empiricism only, an efficient way of predicting and preselecting the most promising candidate materials and experiments is highly desirable. The development of efficient and accurate first-principles simulation methods based on quantum mechanics over the last decades enabled virtual experiments with compounds which have not even been synthesized before. With these techniques, we are able to get insights into the structure, properties and chemical reactivity of substances. We gain knowledge about reaction mechanisms and about the properties determining application performance. Very often, results of the simulations are complementary to the available experimental experience. A clever combination of scientific modeling and experiments is the key to success. In this talk, some examples are given about the application of quantum mechanics to real-world chemical problems in an industrial context.