MO 18: High-Resolution Spectroscopy

Time: Thursday 14:30–16:30 Location: MO-H5

Invited Talk MO 18.1 Thu 14:30 MO-H5

High-resolution spectroscopic studies of transient carbon-rich species — •Sven Thorwirth, Oskar Asvany, and Stephan Schlemmer — I. Physikalisches Institut, Universität zu Köln

Carbon-rich material is of importance in diverse scientific areas such as material science, structural chemistry, theoretical- and astrochemistry. In space, carbon-rich molecular chains both in their neutral and charged forms are abundant ingredients of molecular clouds and circumstellar shells. In this talk, recent efforts towards spectroscopic characterization of neutral and positively charged carbon-rich species harboring selected heteroelements will be presented. Neutral chains were studied at high spectral resolution using a combination of laser ablation production and infrared laser spectroscopy. Positively charged species were observed as products of electron impact ionization of precursor gases using infrared/millimeter-wave techniques and action spectroscopy in 22-pole ion trap instruments. Spectroscopic analyses were guided and facilitated by high-level quantum-chemical calculations.

MO 18.2 Thu 15:00 MO-H5

High-resolution electronic spectroscopy of phthalocyanines in the gas phase — •Florian Schlaghaufer and Alkwin Slenczka — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93053 Regensburg, Germany

The spectral shape of the zero-phonon-line in the electronic and Stark spectra of organic molecules such as phthalocyanines [1] and porphine [2] and their clusters with small atoms and molecules (e.g. H_2O, Ar) recorded in superfluid helium nanodroplets is determined by pure molecular contributions and the influence of the helium environment. Since the analysis of such line shapes is not straightforward, corresponding gas phase studies are essential for dissecting helium induced spectral features from molecular rotor fingerprints.

This talk will give an overview of our recent experimental proceedings on spectroscopy of jet cooled phthalocyanines as well as data analysis used to obtain information on structure and polarity of the molecular systems for both the ground and the electronically excited state. To our best knowledge phthalocyanine is the largest molecule ever studied with respect to its rotational degrees of freedom so far.

Ultimately, this project heads for a better understanding of microsolvation and the dynamics of electronic excitation of molecules inside superfluid helium nanodroplets via combined gas phase and helium droplet investigations.

[1] J. Chem. Phys. 2018, 148, 144301.
[2] J. Chem. Phys. 2018, 149, 244306.

MO 18.3 Thu 15:15 MO-H5

Vibronic couplings in Serotonin — •Christian Brand[1,2] and Michael Schmitt[1] — [1]Heinrich-Heine University, Institute of Physical Chemistry I — [2]German Aerospace Center, Institute of Quantum Technologies

We discuss vibronic couplings between the lowest two excited singlet states (L_a and L_b) of the neurotransmitter serotonin. In this derivative of indole, we expect a large energy gap between the two states of ≈ 3300 cm^{-1} and thus only weak couplings. Nevertheless, using rotationally resolved electronic spectroscopy, we observe a mode-dependent rotation of the L_b transition dipole moment vector in the direction of the L_a. This study bridges the gap between strong and completely suppressed couplings, as previously observed for other indole derivatives.

[1] C. Brand and M. Schmitt, J. Mol. Struct. **1250**, 131819 (2022)

MO 18.4 Thu 15:30 MO-H5

High resolution continuous wave spectroscopy of the $A\,^2\Sigma^+ \leftarrow X\,^2\Pi_{3/2}$ transition in nitric oxide — •Patrick Kaspar[1], Fabian Munkes[1], Philipp Neufeld[1], Lea Ebel[1], Yannick Schellander[2], Robert Löw[1], Tilman Pfau[1], and Harald Kübler[1] — [1]5. Physikalisches Institut and Center for Integrated Quantum Science and Technology IQST, Universität Stuttgart — [2]Institut für Großflächige Mikroelektronik, Universität Stuttgart

Within the scope of the development of a new kind of gas sensor[1,2], we employ Doppler-free saturated absorption spectroscopy on the $A\,^2\Sigma^+ \leftarrow X\,^2\Pi_{3/2}$ transition in nitric oxide (NO) for different total angular momenta J on the P_{12} branch. Spectroscopy is performed in continuous wave operation at 226 nm in a 50 cm long through-flow cell. Via phase sensitive detection by a lock-in amplifier the hyperfine structure of the $X\,^2\Pi_{3/2}$ state of NO is partially resolved. The data is compared to previous measurements [3], showing good agreement. Investigation of the dependence of the spectroscopic feature on power and pressure, should yield hyperfine constants, natural transition linewidth and the collisional cross-section between NO molecules.

[1] P. Kaspar et. al., OSA Optical Sensors and Sensing, 19-23 July, 2021
[2] J. Schmidt et. al., Appl. Phys. Lett. **113**, 01113 (2018)
[3] W.L. Meerts and A. Dymanus, J. of Mol. Spec. 44, 320-346 (1972)

MO 18.5 Thu 15:45 MO-H5

Spectral learning for (ro-)vibrational calculations of weakly-bound molecules — •Yahya Saleh[1,2], Jannik Eggers[1,2], Vishnu Sanjay[6], Andrey Yachmenev[1,3], Armin Iske[2], and Jochen Küpper[1,3,4,5] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Mathematics, Universität Hamburg, Hamburg, Germany — [3]Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany — [4]Department of Physics, Universität Hamburg, Hamburg, Germany — [5]Department of Chemistry, Universität Hamburg, Hamburg, Germany — [6]Gran Sasso Science Institute

Weakly-bound complexes of organic molecules with water play diverse roles in various fields ranging from biology to astrochemistry. Planning experiments requires accurate quantum mechanical calculations of (ro-)vibrational energies up to dissociation, which is a challenging task for these systems. Standard predictions for these problems represent the wavefunctions as a linear combination of some fixed basis set. The quality of the predictions deteriorate for highly-excited states. Moreover, the computational costs scale poorly with the dimension of the problem.

We present a nonlinear variational framework to simultaneously compute multiple eigenstates of quantum systems using neural networks. The proposed framework is shown to model excited states more accurately and is believed to scale better with the size of the system. We also present numerical analysis' results and convergence guarantees of the proposed approach.

MO 18.6 Thu 16:00 MO-H5

SFQEDtoolkit: a high-performance library for modeling strong-field QED effects in relativistic laboratory astrophysics — •Samuele Montefiori and Matteo Tamburini — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany

Given the need of modeling strong-field QED (SFQED) processes such as high-energy photon emission and electron-positron pair creation in forthcoming relativistic laboratory experiments at ultrahigh fields, we have developed an open source library that allows the implementation of SFQED effects in existing Monte Carlo and Particle-In-Cell (PIC) codes. The SFQEDtoolkit library is primarily designed to simultaneously achieve high performance and high accuracy in modeling the functions that describe SFQED processes within and beyond the locally constant field approximation (LCFA).

MO 18.7 Thu 16:15 MO-H5

Auger electron spectroscopy of Fulminic acid, HCNO — •Marius Gerlach[1], Tobias Preitschopf[1], Emil Karaev[1], Heidy Lara[1], Dennis Mayer[2], John Bozek[3], Reinhold Fink[4], and Ingo Fischer[1] — [1]Universität Würzburg, 97074 Würzburg, Germany — [2]Universität Potsdam, 14476 Potsdam-Golm — [3]Synchrotron SOLEIL, 91192 Gif Sur Yvette, France — [4]Universtiät Tübingen, 72076 Tübingen

In 2009 fulminic acid, HCNO, was first detected in space in the three starless cores B1, L1544 and L183.[1] The isomer isocyanic acid, HNCO, is also ubiquitous in interstellar systems.[2] Due to their composition of Hydrogen, Carbon, Nitrogen and Oxygen these molecules have been proposed to have a prebiotic role as intermediates for organic life. Investigating the interaction of these molecules with X-ray radiation is critical in understanding their fate in space.

As such, we present the gas phase auger electron spectra of fulminic acid which were recorded at the PLEIADES beamline at the Synchrotron SOLEIL in France. Fulminic acid was synthesized by preparative pyrolysis.[3] The spectra are compared to theoretical simulations and previously recorded spectra of isocyanic acid.

[1] N. Marcelino, J. Cernicharo, B. Tercero, E. Roueff, Astrophys. J., 2009, 690, L27-L30.

[2] Nguyen-Q-Rieu, C. Henkel, J. M. Jackson, R. Mauersberger, Astron. Astrophys., 1991, 241, L33.

[3] C. Wentrup, B. Gerecht, H. Briehl, Angew. Chem. Int. Ed., 1979, 18, 467-468.