MOLECULAR QUANTUM SCIENCE & TECHNOLOGY

31st of January – 2nd of February 2024
Atominstitut, TU Wien

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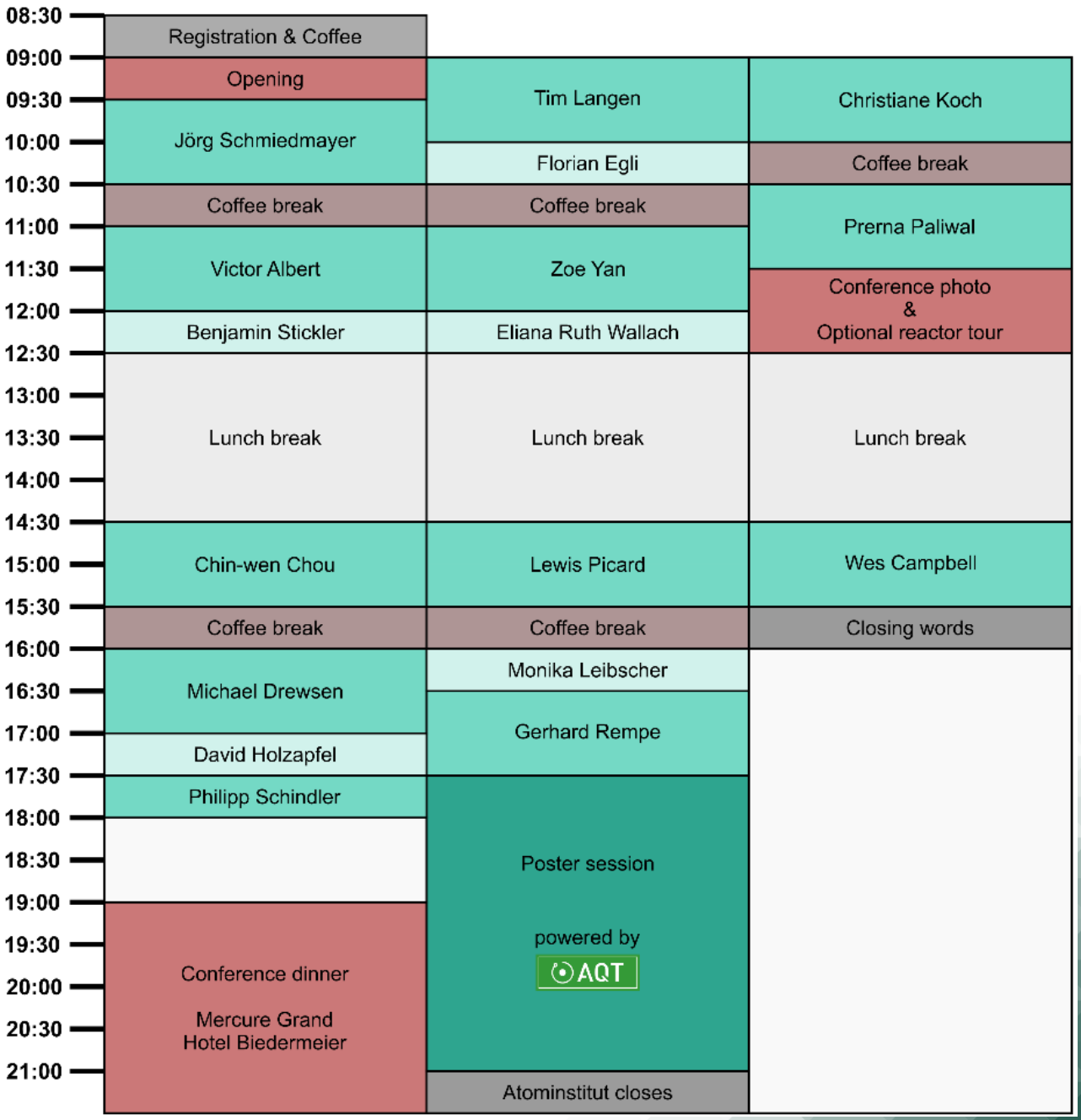
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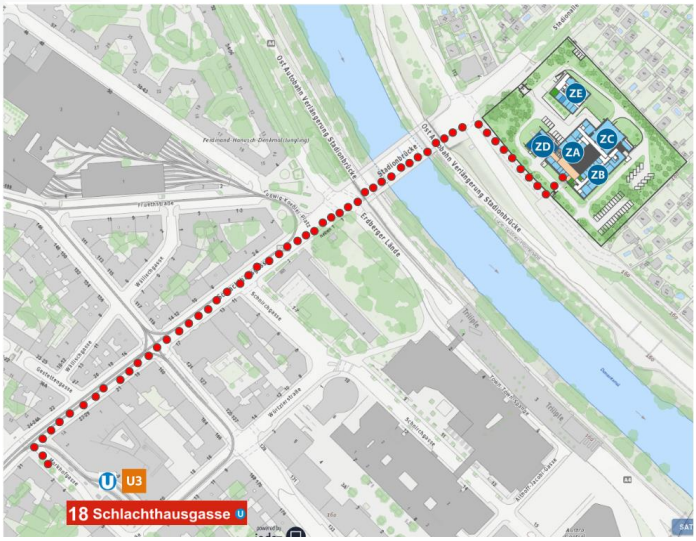

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Stadionallee 2, 1020 Vienna, Austria
Telephone: +43 1 58 801 141 11
Website: www.tuwien.at/phy/ati

An address used earlier (1020 Vienna, Schüttelstraße 115) may still circulate but it designates the same building.

Directions:

1. Take the underground **U3** directed **“Simmering”** from city center to **Schlachthausgasse** station.
2. Walk up the **Markhofgasse Exit**.
3. Get on one of the buses **77A** (direction Lusthaus) or **80A** (direction Praterstern) for two stations to **Schüttelstraße** station.
4. Or you can walk via Schlachthausgasse and Stadionbrücke, this will take about 10 minutes.

INVITED TALKS (DAY 1)

09:30 Jörg Schmiedmayer, *VCQ, TU Wien & WPI*
Hybrid Quantum Systems: Connecting Spins and Photons

Many applications of quantum physics require seemingly contradicting properties to be realized in the same system or device. Hybrid quantum platforms promise to pool the strengths of the individual systems to compensate for their weaknesses to achieve what a single platform cannot. Over the years a large variety of such Hybrid Quantum Systems was developed, tested, and applied in a long series of fundamental research and towards real-world applications [1]. In my talk, I will concentrate on systems connecting photons and spins. I will briefly discuss optical photons connected to atomic ensembles and then concentrate on spins coupled to microwave photons in superconducting quantum circuits. With electron spins in diamond strongly coupled to microwave photons in superconducting cavities I will highlight how such a hybrid system can be employed to probe the physics of the electron spins and the related magnetic cavity QED. Finally, I will discuss a radical new system: atomic and molecular impurities embedded in quantum solids. These noble gas spin-0 Van der Waals crystals are magnetically quiet and their soft nature provides a weakly interacting environment that aims to mitigate the matrix-impurity interaction. I will present our recent progress on microwave measurements with doped cryogenic crystals and discuss the path towards strong coupling of a single molecule to a superconducting resonator.
[1] Quantum Technologies with Hybrid Systems; G. Kurizki, et al. PNAS 112, 3866 (2015)

11:00 Victor Albert, *NIST Maryland and University of Maryland College Park*
Entanglement, geometry, and topology of molecular position states

We formulate a notion of conjugacy between position and momentum for rotational and nuclear-spin states of arbitrary rigid closed-shell molecules. Taking in molecular geometry and nuclear-spin data, our framework yields admissible position and momentum states, inter-convertible via a generalized Fourier transform. We classify molecules into three types — asymmetric, rotationally symmetric, and perrotationally symmetric — with the last type having no macroscopic analogue due to nuclear-spin statistics constraints. We identify two predominant features of perrotationally symmetric state spaces that are independent of any Hamiltonian and that are induced solely by symmetry and spin statistics. First, many molecular species admit intrinsic rotation-spin entanglement that cannot be broken without transitioning to another species. Second, adiabatic changes in position realize naturally robust operations in the form of an Abelian or even non-Abelian monodromy, akin to what is achieved by braiding anyonic quasiparticles or realizing fault-tolerant quantum gates.

INVITED TALKS (DAY 1)

12:00 Benjamin Stickler, *Ulm University*

Surface-induced rotational decoherence of a two-ion planar rotor

Quantum rotors promise unique advantages for quantum sensing, quantum simulation, and quantum information processing. For future applications, understanding their dynamics in the presence of ambient environments and decoherence will be critical. In this contribution, I will present the theoretical framework for modelling surface-induced decoherence and heating of charged rotors near metallic surfaces [1]. I will then use this framework to describe recent measurements of rotational decoherence with a quantum planar rotor realized by two trapped ions [2]. We find excellent agreement between experiment and theory.

[1] Martinetz, Hornberger, and Stickler, Surface-induced decoherence and heating of charged particles, PRX Quantum 3, 030327 (2022)
[2] Glikin, Stickler, Tollefsen, Mouradian, Yadav, Urban, Hornberger, Haeffner, Systematic study of rotational decoherence with a trapped-ion planar rotor, arXiv: 2310.13293 (2023)

14:30 Chin-wen (James) Chou, *NIST Boulder*

Quantum state control of single molecular ions

A large variety of molecular species exist, each with distinct properties and featuring a high-dimensional rotational-vibrational state space. Specific molecules could offer certain advantages in quantum science and technology (QST). However, the complexity of molecular state spaces makes it challenging to prepare, control, and read out molecular quantum states with high fidelity, a prerequisite for harnessing their diversity for QST. The Ion Storage group at NIST is extending control over a growing number of quantum states in single molecular ions by incorporating laser cooling and trapping techniques, frequency comb technology, and quantumlogic spectroscopy protocols. Quantum states of a single molecular ion can be prepared, coherently manipulated, and detected nondestructively, enabling rotational-vibrational spectroscopy with better than part-per-trillion resolution and atom-molecule quantum entanglement. This approach is applicable to a broad range of molecular ion species that can be selected for specific applications, such as transducing quantum information between stationary and flying qubits. We are also exploring new opportunities in physics and chemistry offered by the rich structure and abundance of molecular species.

*In collaboration with A. Collopy, Y. Lin, C. Kurz, M. E. Harding, P. N. Plessow, T. Fortier, S. Diddams, Y. Liu, Z. Liu, J. Schmidt, D. Chaffee, B. Margulis, D. Hume, D. R. Leibrandt, and D. Leibfried.

16:00 Michael Drewsen, *Aarhus University*

Ground-State Cooled Molecular Ions: Unresolved Photon Recoil Spectroscopy and Tests of Continuous Spontaneous Localization Models

Trapped and laser-cooled atomic ions have for many years been representing one of the leading platforms for the development of practical quantum computers and simulators, as well as other quantum technology (QT) devises. In this contexts, smaller molecular ions with richer but still manageable energy level structures can potentially lead to improved performances. Conversely, QT tools developed for atomic ions can beneficially be applied in investigations based on molecular ions, as has recently been demonstrated with small diatomic molecular ions. In my presentation, I will discuss how I see such QT tools applied in two very different types of experimental studies with complex molecular ions, namely in photon recoil spectroscopy in the unresolve motional sideband regime, and in test of quantum mechanics at the mesoscopic scale.

INVITED TALKS (DAY 1)

17:00 David Holzapfel, *ETH Zurich*

Quantum logic spectroscopy of the hydrogen molecular ion

I will present our latest results, implementing pure quantum state preparation, coherent manipulation, and non-destructive state readout of the hydrogen molecular ion H_2^+.
The hydrogen molecular ion H_2^+ is the simplest stable molecule, and its structure can be calculated ab-initio to high precision. However, challenging properties such as high reactivity, low mass, and the absence of rovibrational dipole transitions have thus far strongly limited spectroscopic studies of H_2^+.
We trap a single H_2^+ molecule together with a single beryllium ion using a cryogenic Paul trap apparatus, achieving trapping lifetimes of 11h and ground-state cooling of the shared axial motion. With this platform we have recently implemented *Quantum Logic Spectroscopy* of H_2^+.
We utilize helium buffer-gas cooling to prepare the lowest rovibrational state of ortho-H_2^+ (rotation $L = 1$, vibration $\nu = 0$). We combine this with quantum-logic operations between the molecule and the beryllium ion for preparation of single hyperfine states and non-destructive readout. Furthermore, we have demonstrated Rabi flopping on one hyperfine transition.
Our results pave the way to many high-precision spectroscopy studies of H_2^+ which will enable tests of theory, metrology of fundamental constants, and the implementation of an optical molecular clock based on the simplest molecule.

17:30 Philipp Schindler, *University of Innsbruck*

Quantum technologies with molecular ions using quantum logic

Full quantum control over individual molecules is the key requirement to enable molecular quantum technologies. Recently, quantum logic spectroscopy has paved the way to impressive quantum control of single molecular ions. In order to increase the complexity of controllable molecular ions, the existing techniques need to be adapted. I will discuss viable extensions of existing quantum logic techniques in ion traps using ultrafast laser pulses in conjunction with projective subspace measurements. Furthermore, I will present a method to implement quantum error correction primitives using the recently presented absorption/emission using the toolbox available in current ion trap experiments.

INVITED TALKS (DAY 2)

09:00 Tim Langen , *TU Wien & WPI*

Laser cooling of barium monofluoride

In the first part of my talk I will report on our progress towards laser cooling of BaF molecules. Due to its high mass, resolved hyperfine structure in the excited state and branching losses through intermediate states, this molecular species is notoriously difficult to cool, but it shows high promise for various types of precision measurement applications. In the second part, I will discuss the new possibilities that bulk molecular Bose-Einstein condensates may open up for dipolar many-body physics in the near future. Building on our work on dipolar droplets and supersolids that form from weakly dipolar atoms, I will show how ultracold molecules and microwave shielding can provide fundamentally new insights into these exotic states of matter.

10:00 Florian Egli, *Max Planck Institute of Quantum Optics*

Using Non-linear Dissociation Processes of BeH^+ for the Alignment of the Laser Pulse Overlap in XUV Frequency Comb Spectroscopy of He+

The energy levels of hydrogen-like atoms and ions are accurately described by bound-state quantum electrodynamics (QED). With spectroscopic measurements of hydrogen and hydrogen-like atoms, the Rydberg constant and the proton charge radius can be determined. The comparison of the physical constants obtained from different combinations of measurements serves as a consistency check for the theory. The hydrogen-like He^+ ion is an interesting spectroscopic target for QED tests. Due to their charge, He^+ ions can be held nearly motionless in the field-free environment of a Paul trap, providing ideal conditions for high-precision measurements. The 1S-2S two-photon transition in He^+ can be directly excited by an extreme-ultraviolet frequency comb at 60.8~nm generated by a high-power infrared frequency comb using high-order harmonic generation (HHG). In order to perform Doppler-free spectroscopy on the 1S-2S transition, the frequency comb is split into double pulses which are overlapped at the ions. As a signal for the pulse overlap alignment, we investigate non-linear dissociation processes of BeH^+. The processes discussed here are using 204~nm and 255~nm light, which can be generated from our infrared frequency comb.

INVITED TALKS (DAY 2)

11:00 Zoe Yan, *University of Chicago*

Quantum correlations in a many-body system of polar molecules

Ultracold molecules have promising applications in the fields of quantum computing and simulation of many-body systems. Central to these applications is the ability to detect and manipulate the quantum state of individual molecules. I will describe the development of a novel apparatus for imaging single diatomic molecules in an ultracold gas prepared in the ground electronic, rovibrational and hyperfine state, performed at Princeton University. We used this capability to measure quantum correlations due to the bosonic statistics of the molecules or due to entanglement mediated by dipolar interactions. As an example of a potential application, I will discuss our study of out-of-equilibrium dynamics in tunable quantum spin models and measurements of the evolution of spatial correlations during the ensuing thermalization process.
Looking ahead, I will describe efforts for next-generation molecular gas experiments at the University of Chicago involving potassium-silver molecules. These 'ultrapolar' molecules are capable of dipolar-mediated entanglement approaching MHz level speeds, presenting interesting opportunities for quantum simulation and information.

12:00 Eliana Ruth Wallach, *Technion - Israel Institute of Technology*

Toward Parity Violation Measurement in Trapped Chiral Molecular Ions

Every chemistry student learns that chiral molecules have two enantiomers - mirror image configurations. However, parity symmetry that is broken by the weak nuclear force, puts this claim into question, predicting a still-unmeasured slight energy difference between both enantiomers.
We are building an experiment to measure PV in cold trapped chiral molecular ions, namely $CHDBrI^+$, which is predicted to have an enhanced vibrational PV shift (JCP, Chem. Comm., 2023). State-selective, near-threshold photoionization will be used to achieve an internally cold ensemble of molecular ions.
Once trapped, PV can be measured in a mixed ensemble of chiral molecules, using our scheme which embeds Ramsey spectroscopy within the 3-wave mixing method, used to separate enantiomers into specific rotational states (PRX 2023). The vibrational PV shift is extracted by taking the difference between the enantiomer-specific Ramsey signals that are imprinted onto the molecules' rotational populations.
The resolved simultaneous readout of the ro-vibrational states will be achieved by observing the velocities of photofragments. Our unique ion trap, which is coupled to a velocity map imaging detector, is designed to have ~2m/s resolution, sufficient to resolve individual rotational states.
We will discuss our progress in this young experiment, including our first steps commissioning the setup.

INVITED TALKS (DAY 2)

14:30 Lewis Picard, *Harvard University*

Millisecond-scale dipolar exchange of rotational excitation between individual molecules in optical tweezers

The ability to engineer long-range interactions between physically separated qubits is the keystone requirement for any experimental quantum information platform. Ultracold dipolar molecules can interact at long-range by virtue of their permanent molecule-frame dipole moments, which can mediate resonant exchange of molecular rotations between molecules at distances of several micrometers. Our platform consists of ultracold NaCs molecules adiabatically assembled from their constituent atoms in optical tweezers. By rotating the tweezer polarization to a specific magic ellipticity, we are able to isolate a pair of rotational states in the molecule from trap-induced light shifts, allowing us to encode a qubit in them with a coherence time of up to 250 ms. In this talk I will present our realization of controlled dipole-mediated exchange of excitations between neighboring molecular qubits with an exchange time of less than 1 ms at a separation of 1.6 μm. I will further discuss how these coherent rotational interactions can be used to generate entanglement for a range of quantum information and simulation experiments using this platform.

16:00 Monika Leibscher, *Freie Universität Berlin*

Quantum control of ro-vibrational dynamics in randomly oriented molecules

Controlling molecular rotation by external field has many applications ranging from quantum information to enantio-selective manipulation of chiral molecules. The random orientation of molecules in the gas phase which is reflected in the degeneracy of the rotational spectrum poses a challenge for the control of molecular rotation. We present a graphical method to analyze the controllability of a quantum asymmetric top and to determine the number, polarization and frequencies of the external fields which are required to fully control the rotational dynamics of randomly oriented molecules [1,2]. Moreover, we show that the creation of vibrational coherences in randomly oriented molecules requires control over the rotational degrees of freedom. As an example, we demonstrate the excitation of temporary chiral vibrational states in randomly oriented achiral molecules [3].

[1] M. Leibscher, E. Pozzoli, C. Pérez, M. Schnell, M. Sigalotti, U. Boscain, C. P. Koch, Commun. Phys. 5, 110 (2022).
[2] E. Pozzoli, M. Leibscher, M. Sigalotti, U. Boscain and C. P. Koch, J. Phys. A: Math. Theor. 55, 215301 (2022).
[3] M. Leibscher, E. Pozzoli, A. Blech, M. Sigalotti, U. Boscain, C. P. Koch, arXiv:2310.11570 (2023)

INVITED TALKS (DAY 2)

16:30 Gerhard Rempe, *Max Planck Institute of Quantum Optics*
TBD

TBD

INVITED TALKS (DAY 3)

09:00 Christiane Koch, *Freie Universität Berlin*

Quantum effects in controlled molecular dynamics

Molecular quantum science and technology hinges on the exploitation of quantum effects. I will discuss three examples of molecular dynamics where quantum effects are particularly pronounced. (i) Quantum scattering resonances attest to the wave nature of matter. They result in distinct quantum fingerprints in collision cross sections [1] and allow for disentangling the isotropic and anisotropic contributions to the inter-particle interaction when probed with rotationally state-selected molecules [2]. (ii) The wave nature of matter also gives rise to phase protection of Fano-Feshbach resonances, a mechanism that protects a bound state from decay despite resonant coupling to a scattering continuum. For rare gas diatomic ions, it results in predissociation lifetimes spanning four orders of magnitude, in good agreement with experimental measurements [3]. (iii) Yet another signature of quantum mechanics is found in selection rules governing the light-matter interaction. They follow from the quantization of molecular rotations which occupy the low-energy part of the molecular spectrum and are ideally suited for quantum control [4]. I will explain how full control over the dynamics in degenerate rotational subspaces can be achieved by suitable combinations of electric fields [5] and discuss implications for state preparation and quantum gate implementations.

[1] Margulis et al., Science 380, 77 (2023).
[2] Klein et al., Nature Physics 13, 35 (2017).
[3] Blech et al., Nature Comm. 11, 999 (2020).
[4] Koch, Lemeshko & Sugny, Rev. Mod. Phys. 91, 035005 (2019).
[5] Leibscher et al., Commun. Phys. 5, 110 (2022).

10:30 Prerna Paliwal, *University of Basel*

Quantum-logic control of complex molecular ions for applications in molecular and chemical physics

Over the past years, the coherent manipulation of single isolated quantum systems such as atoms, ions, superconducting circuits, and quantum dots has advanced greatly and yielded important applications in the fields of quantum metrology, quantum sensing, and quantum computing. Recently, extending and applying quantum technologies to molecules has become one of the prime goals of the quantum physics community. However, their complex internal structure and lack of cycling transitions make it difficult to cool, control, and manipulate them. In our lab, we co-trap a single molecular ion together with an atomic ion which acts as a coolant to cool the molecule translationally as well as a messenger for the internal state identification of the molecule without destroying it. The information of the complex molecular ion is mapped onto an easily addressable atomic ion from where it is read out [1-5]. I will talk about the quantum-non-demolition detection of the rovibrational state of single nitrogen ions which is a crucial step towards their coherent manipulation. This method allows us to go beyond the state-of-the-art and prepare molecular ions in well-defined hyperfine-Zeeman states. I will also discuss the extension of our technique to polyatomic ions to lay the foundations for the exploration of their spectroscopy and molecular dynamics.

[1] Schmidt et al., Science 309, 749 (2005).
[2] Hume et al., PRL 107, 243902 (2011).
[3] Meir et al., Faraday Discuss. 217, 561 (2019).
[4] Sinhal et al., Science 367, 1213 (2020).
[5] Najafian, et al., Nat. Commun. 11, 4470 (2020).

INVITED TALKS (DAY 3)

14:30 Wes Campbell, *University of California Los Angeles*
Optical cycling in aromatic molecules

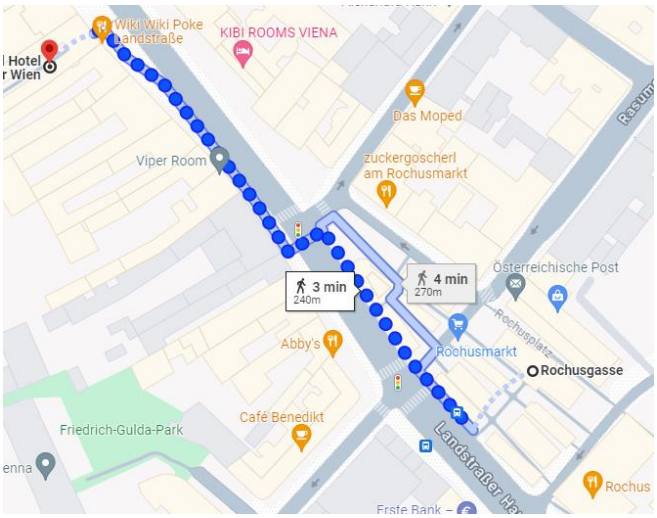
Optical cycling allows laser-induced fluorescence to be repeated many times with a nearly deterministic final internal state. These transitions are useful for laser-driven applications such as Doppler cooling and quantum state preparation and detection of qubits. I will discuss recent progress toward endowing molecules as large as polycyclic arenes with optical cycling centers. Thinking ahead, it is worthwhile to consider and how this progress may continue even when the species involved are so large that rotational lines are no longer optically resolved. This leads to a direct rotational analogue of laser cooling of atomic translation, and connections between the two can provide insight about each.

CONFERENCE DINNER

Wednesday, 31.01.2024 at 19:00

Der Sünnhofkeller of Mercure Grand Hotel Biedermeier Wien

Landstraßer Hauptstraße 28,
1030, Vienna, Austria



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1. Take the underground **U3** directed **“Ottakringer”** to **Rochusgasse** station.
2. Walk up the **Rochusmarkt Exit**.
3. Walk via Landstraßer Hauptstraße and turn left into Sünnhof, this will take about 3 minutes.

POSTER SESSION

Thursday, 01.02.2024

at 17:30 – 21:00

ATI, 1st floor hallway

Snacks&Beverages will be provided

You may set up your poster on Wednesday and leave it up for the duration of the conference. It must be taken down by 13:00 on Friday.

Download the book of abstracts here!

LUNCH OPTIONS

Restaurants

ETAP, Turkish restaurant
10:00 – 15:00
Thomas-Klestil-Platz 2, 1030 Wien
https://www.etap-restaurant.at/

8 min walk from the conference venue

GUSTO, Takeout restaurant
Mo-Th: 11:00 – 14:00, Fr: 11:00 – 13:00
Thomas-Klestil-Platz 11, 1030 Wien
http://www.gusto.co.at/

11 min walk from the conference venue

Lucky Kitchen, Asian restaurant
10:00 – 22:00
Würtzlerstraße 11, 1030 Wien
https://www.luckykitchen.at/

7 min walk from the conference venue

LUNCH OPTIONS

Supermarkets

BILLA
07:15 – 19:30
Schnirchgasse 9, 1030 Wien

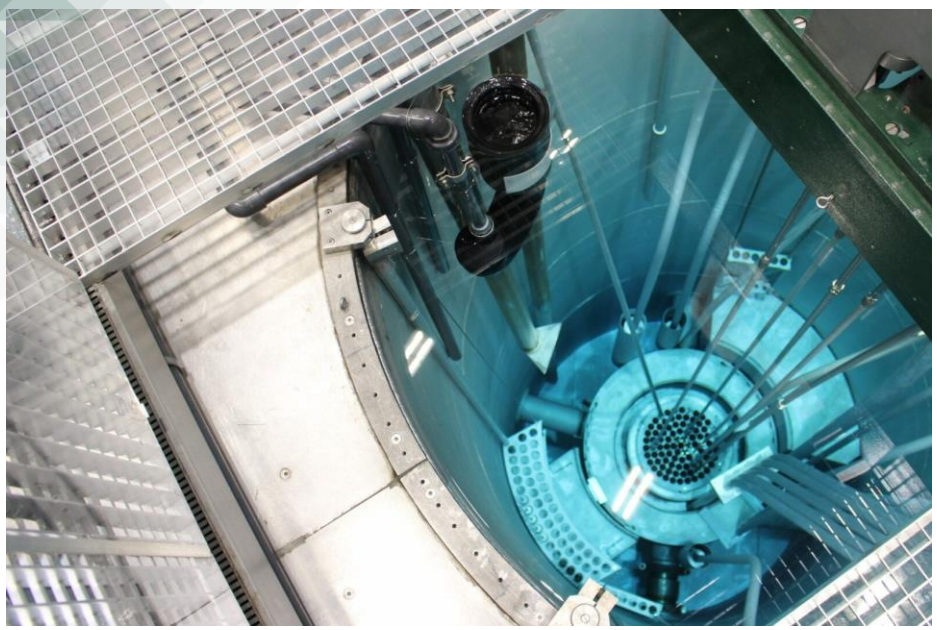
6 min walk from the conference venue

SPAR
07:40 – 20:00
Schlachthausgasse 15/17, 1030 Wien

5 min walk from the conference venue

More restaurants and supermarkets are available around the Atominstitut, you can always opt for takeout and eat at the conference venue.

REACTOR TOUR



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Friday, 02.02.2024 at 11:30

Austria’s only nuclear research facility is the **Atominstitut** in Vienna’s Prater. It is an important link to the European scientific environment and is acknowledged as a highly specialized international training institution due to its near proximity to the International Atomic Energy Agency IAEA and major European research facilities.

TRIGA Mark II research reactor opened in 1962 and is now dedicated to today's broad range of research and education ranging from very fundamental questions about symmetries and interactions in nuclear and particle physics to neutron-, atomic-, quantum-physics.

Please, signed up for the tour at the registration desk!

CONTACTS

From left to right: Brandon Furey, Stefan Walser, Elena Redchenko, Andrew Kanagin

You can always contact us using the conference email address: mqst2024@tuwien.ac.at

Or contact one of the organizers directly:

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Gas emergency	128
Police	133
Emergency doctor	141
Crisis hotline	142
Ambulance service	144
Poison centre	01 406 43 43

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https://mqst2024.conf.tuwien.ac.at/