

# THU 4: Precise Quantum Molecules: Contributed Session to Symposium

Time: Thursday 14:15–15:15

Location: ZHG004

THU 4.1 Thu 14:15 ZHG004

**Floquet-Engineering of Bound States in the Continuum** —  
•ALEXANDER GUTHMANN, LOUISA MARIE KIENESBERGER, FELIX  
LANG, and ARTUR WIDERA — Physics Department and Research Cen-  
ter OPTIMAS, University of Kaiserslautern-Landau

Scattering resonances play a pivotal role in quantum phenomena, from nuclear reactions to ultracold atomic collisions. Our recent work has demonstrated that periodic modulation of the magnetic field can be used to induce Floquet-Feshbach resonances in a two-component gas of fermionic lithium-6 [1], enabling precise control over resonance positions and suppression of inelastic losses.

This talk will focus on a new application of this technique: the realization of Bound States in the Continuum (BICs) through interference at an avoided crossing between two Floquet-engineered resonances. BICs are exotic quantum states that remain localized despite existing within the energy continuum of scattering states. As first predicted by Friedrich and Wintgen [2], such states can emerge through destructive interference at an avoided crossing of two resonances. While BICs have been realized in photonic and acoustic platforms, their observation in a true molecular dimer system has remained a longstanding challenge. [1] A. Guthmann, F. Lang, L. M. Kienesberger, S. Barbosa, A. Widera, arXiv 2503.05454 (2025).

[2] H. Friedrich and D. Wintgen, Phys. Rev. A 32, 3231 (1985).

THU 4.2 Thu 14:30 ZHG004

**Near-complete chiral selection in rotational quantum states** —  
•ELAHE ABDIHA, JUHYEON LEE, SHILPA YADAV, SEJUN AN, BORIS  
G SARTAKOV, GERARD MEIJER, and SANDRA EIBENBERGER-ARIAS —  
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many

In our work, we accomplish near-complete chiral selection in rotational quantum states [1]. Beyond mere chiral analysis, enantiomer-specific state transfer (ESST) enables the control and manipulation of chiral molecules at the quantum level. We overcome previous limitations of ESST by applying UV laser and microwave radiation to a triad of rotational states connected to the absolute ground state. Our experimental results show that 96% state-specific enantiomeric purity can be obtained from a racemic mixture, in an approach that is universally applicable to all chiral molecules of C1 symmetry. Our work has the potential to significantly advance the experimental methods to measure parity-violation effects in chiral molecules [4].

We will also present our ongoing efforts to address the intrinsic limitation of ESST due to orientational degeneracy of rotational states by incorporating theoretically tailored microwave pulse schemes [5].

[1] Lee et al. Nat. Commun. 15, 7441 (2024)

[2] Eibenberger et al. Phys. Rev. Lett. 118, 123002 (2017)

[3] Pérez et al. Angew. Chem. Int. Ed. 56, 12512 (2017)

[4] Erez et al. Phys. Rev. X, 13, 041025, (2023)

[5] M. Leibscher et al. Commun. Phys. 5, 110 (2022).

THU 4.3 Thu 14:45 ZHG004

**Observation of rovibrational state interference in molecule-surface collisions** — •CHRISTOPHER REILLY<sup>1</sup>, DANIEL J. AUERBACH<sup>2</sup>, and RAINER D. BECK<sup>1</sup> — <sup>1</sup>EPFL, Lausanne, Switzerland — <sup>2</sup>MPINAT, Göttingen, Germany

While for all but the lightest molecular species the collisional generation and absorption of surface phonons typically obscures the ultimately quantum mechanical nature of molecule-surface collisions, a special continuous reflection symmetry in the interaction between methane and a gold surface permits observation of striking interference effects in the distribution of quantum states populated in the scattering event. Moreover, this interference effect is unique to molecules with some minimum amount of internal structure and is thus absent for the simpler molecular species typically studied.

Using laser-based quantum state preparation and detection, we are able to observe a novel form of high-contrast destructive interference between rovibrational states in molecule-surface scattering[1]. By exciting molecules to or from a rovibrational state of zero angular momentum, we prepare a state of pure reflection parity, and when probing the scattered molecules we find an almost total absence of population in states of the opposite parity. Reflection parity conservation is observed in both the ground and excited vibrational states, with contrast ratios approaching 100:1. High-contrast interference is also observed for rare vibrational relaxation events, shedding light on their microscopic mechanism.

[1] Reilly et al., Science 387, 962 (2025)

THU 4.4 Thu 15:00 ZHG004

**Quantum-mechanical calculations for million-atom biological systems** — •LUC WIENERS and MARTIN E. GARCIA — Institut für  
Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel,  
Germany

Quantum-mechanical first-principles calculations are commonly only used for systems containing a few hundred atoms which leaves biological systems with thousands or millions of atoms inaccessible. In this study we show a new algorithm for the Hartree-Fock method combined with a divide-and-conquer approach which enables calculations of million-atom biological systems, including a whole bacteriophage in a solution which in total contains 45 million atoms.

The high computational speed also allows the calculation of spectra for systems with hundreds to a few thousand atoms. This is used to compute absorption spectra for proteins, DNA and medications. Additionally, Hartree-Fock atomic energies are found to coincide with AlphaFold's pLDDT confidence score for protein structure predictions, showing a connection between first-principle calculations and protein structure assessment.

We anticipate that the presented methods open a pathway to fully quantum-mechanical investigations including more accurate molecular dynamics simulations and theoretical predictions of spectral properties for systems in biology and medicine.