



## Physical Sciences Seminar

# Recent Developments and Future Challenges for Molecular Quantum Theory

**Edit Mátyus (Eötvös Loránd University)**

**Host: Laszlo Erdös**

High-resolution spectroscopy experiments provide us information about the internal motion of molecular systems with an extraordinary detail and precision. Aiming at a quantitative agreement with the experimental data makes it necessary to massively extend our knowledge about the fundamental properties of molecular matter. In this talk, I will report on recent progress along challenging directions of this field. Multiple, coupled, large-amplitude motions in high-dimensional quantum systems are ubiquitous in nature, still quantitative solution of the corresponding Schrödinger equation is extremely challenging. I will point on the main bottlenecks and explain our solution strategy. Coupling in the quantum mechanical motion of the electrons and the atomic nuclei in molecules is thought to be understood by and large. When it comes to a quantitative understanding, even the smallest molecular systems,  $H_2$  and  $H_3^+$ , turn out to be extraordinarily difficult. I will speak about a perturbative and a variational approach to the electron-nucleus problem. For certain energetic and structural ranges, the computations could have been carried out with full rigor, and we are in a position to assess relativistic, quantum electrodynamics, and finite-nuclear size effects in molecules to be compared with the experimental data.

**Tuesday, January 21, 2020 11:00am - 12:00pm**

IST Austria Campus Heinzl Seminar Room / Office Bldg West (I21.EG.101)



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