Thomas Grohmann

Research statement

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Basically, my research focusses on the role of symmetry in molecular quantum theory. In my early works, I was addressing in particular the quantum dynamics of the nuclear spin isomers of molecules in the context of the alignment of rigid molecules and directed motions in non-rigid molecules. These works show how the nuclear spin symmetries determine the response of molecules to laser pulses, and how these differences can be used to design molecular rotors. Later, I extended my research to open quantum systems and molecules with coupled rotations and contortion. Based on a four-dimensional model, I developed criteria that have to be fulfilled for simple descriptions of molecular torsions to be appropriate. Currently, I am working on fundamental questions related to Theoretical Chemistry and Molecular Physics. Specifically, I am investigating how quantum-classical theories, such as classical molecular dynamics simulations, violate fundamental quantum theoretical principles, and I explore what consequences follow from these violations for the interpretation of molecular dynamics simulations, experiments on attosecond chemistry and physics, and molecular structures.

Selected publications

- »Nuclear spin selective laser control of rotational and torsional dynamics«

  Authors Johannes Floß, **Thomas Grohmann**, Monika Leibscher⊛, Tamar Seideman
  published in The Journal of Chemical Physics **136** (2012), pp. 084309

- »On the impossibility of localised states for molecular rotors with cyclic potentials«

  Authors **Thomas Grohmann**⊛, Jörn Manz
  published in Molecular Physics **116** (2018), pp. 2538

- »Nuclear spin blockade of laser ignition of intramolecular rotation in the model boron rotor $^{11}B_{13}^{+}$«

  Authors **Thomas Grohmann**, Dietrich Haase, Donming Jia⊛, Jörn Manz, Yonggang Yang
  published in The Journal of Chemical Physics **149** (2018) pp. 184302

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