

# Recent Results on the Time Dependent Quantum Dynamics of Mode Selective Intramolecular Energy Flow and Tunneling in Polyatomic Molecules and Clusters

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We shall introduce the two major experimental approaches towards intramolecular quantum dynamics and kinetics from spectra, (i) the study of time resolved spectra, which has a long history of many decades, and (ii) deriving time dependent quantum dynamics from highly frequency resolved molecular spectra developed largely in the Zurich group over the last three decades<sup>[1-5]</sup> making use also of developments in the theory of molecular quantum dynamics. We shall then report about recent experimental and theoretical results from our group ranging from femtosecond intramolecular energy flow to picosecond and nanosecond tunneling reactions<sup>[6-8]</sup>, nuclear spin symmetry violation<sup>[9-11]</sup>, and finally time dependent evolution of parity on the time scale of seconds due to electroweak parity violation<sup>[3, 12-18]</sup> including some recent open problems in molecular quantum dynamics<sup>[15]</sup>. The role of successive symmetry breakings in defining different time scales of intramolecular primary processes of kinetics will be emphasized<sup>[3]</sup>.

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## References

- [1] M. Quack, in *COST MOLIM meeting, 10 - 12 October 2016*, Dubrovnik, **2016**. [www.ir.ethz.ch](http://www.ir.ethz.ch)
- [2] M. Quack, *Molecular femtosecond quantum dynamics between less than yoctoseconds and more than days: Experiment and theory*, in *Femtosecond Chemistry, Proc. Berlin Conf. Femtosecond Chemistry, Berlin (March 1993)* (Eds.: J. Manz, L. Woeste), Verlag Chemie, Weinheim, **1995**, pp. 781-818. M. Quack and J. Stohner, *J. Phys. Chem.* **1993**, *97*, 12574-12590
- [3] M. Quack, *Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy*, in *Handbook of High Resolution Spectroscopy, Vol. 1* (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**, pp. 659-722.
- [4] M. Quack, *Molecules in Motion Chimia* **2001**, *55*, 753-758.
- [5] F. Merkt, M. Quack, *Molecular Quantum Mechanics and Molecular Spectra, Molecular Symmetry, and Interaction of Matter with Radiation*, in *Handbook of High-Resolution Spectroscopy, Vol. 1* (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**, pp. 1-55, (see also preface to this Handbook).
- [6] B. Fehrensens, D. Luckhaus, M. Quack, *Chem. Phys.* **2007**, *338*, 90-105.
- [7] S. Albert, P. Lerch, R. Prentner, M. Quack, *Angew. Chem. Int. Ed.* **2013**, *52*, 346-349. S. Albert, Z. Chen, C. Fabri, P. Lerch, R. Prentner, M. Quack, *Mol Phys.* **2016**, DOI:10.1080/00268976.2016.1226444, in press
- [8] R. Marquardt, M. Quack, *Global Analytical Potential Energy Surfaces for High Resolution Molecular Spectroscopy and Reaction Dynamics*, in *Handbook of High-Resolution Spectroscopy, Vol. 1* (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**, pp. 511-549. C. Fabri, R. Marquardt, M. Quack, *Chimia* **2014**, *68* suppl. and in preparation **2016**
- [9] M. Quack, *Mol. Phys.* **1977**, *34*, 477-504.
- [10] C. Manca Tanner, M. Quack, D. Schmidiger, *J. Phys. Chem. A* **2013**, *117*, 10105-10118
- [11] M. Snels, V. Horká-Zelenková, H. Hollenstein, M. Quack, *High Resolution FTIR and Diode Laser Spectroscopy of Supersonic Jets*, in *Handbook of High Resolution Spectroscopy, Vol. 2* (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, **2011**, pp. 1021-1067.
- [12] M. Quack, *Chem. Phys. Lett.* **1986**, *132*, 147-153.
- [13] M. Quack, J. Stohner, M. Willeke, *Annu. Rev. Phys. Chem.* **2008**, *59*, 741-769.
- [14] R. Prentner, M. Quack, J. Stohner, M. Willeke, *J. Phys. Chem. A.* **2015**, *119*, 12805-12822
- [15] M. Quack, *Frontiers in Spectroscopy*, in *Faraday Discuss.*, Vol. 150, **2011**, pp. 533-565.
- [16] P. Dietiker, E. Miloglyadov, M. Quack, A. Schneider, G. Seyfang, *J. Chem. Phys.* **2012**, *143*, 244305-1-24430523.
- [17] S. Albert, I. Bolotova, Z. Chen, C. Fabri, L. Horny, M. Quack, G. Seyfang and D. Zindel, *PCCP* **2016**, *18*, 21976-21993
- [18] S. Albert, F. Arn, I. Bolotova, Z. Chen, C. Fabri, G. Grassi, P. Lerch, M. Quack, G. Seyfang, A. Wokaun, and D. Zindel, *J. Phys. Chem. Lett.* **2016**, *7*, 3847-3853