From Molecular Spectra to Molecules in Motion, Quantum Chemical Kinetics, Laser Chemistry, and Parity Violation in Chiral Molecules

M. Quack[1]

[1]ETH Zurich, Department of Chemistry and Applied Biosciences, 8093 Zurich, Switzerland - martin@quack.ch, www.ir.ethz.CH

Molecular quantum dynamics, the primary processes of molecules in motion, provide the foundation of all chemical processes, covering combustion as an early and still today important use of chemistry by mankind, the chemistry of planetary atmospheres and of interstellar space, of large scale industrial syntheses, catalysis, and also of the microscopic biomolecular processes in the chemistry of life, its persistence and evolution. Spectroscopy with either high frequency or with high time resolution, possibly also with an uncertainty principle limited combination of both, provides the most powerful experimental techniques to study such processes [1-4]. In the lecture we shall provide a tour d'horizon of selected results from five decades of our research with examples such as mode selective intramolecular vibrational energy flow [4-6] and laser chemistry, hydrogen bond dissociation dynamics and rearrangement tunnelling [7-10], as well as stereomutation tunnelling reactions, including quasiadiabatic channel above barrier tunnelling [11,12]. We shall briefly address, how the concepts of approximate symmetries and symmetry breakings allow for deriving from spectra and for understanding fundamental primary processes covering 42 orders of magnitude in time between yoctoseconds and exaseconds [13]and give a short summary of the current status of parity violation in chiral molecules[14-15]. We conclude with the example of the 'molecular quantum chameleon' spectra and dynamics [15-16]demonstrating the fundamental limitations of classical molecular dynamics, and with a hypothesis on a molecular theory of thought and the question of free will ([17] and refs. cited).

[1] M. Quack, F. Merkt, eds., Handbook of High Resolution Spectroscopy, Wiley, Chichester, **2011**.
[2] M. Quack, Frontiers in Spectroscopy,Faraday Discussion **2011**, *150*, 533-565.
[3] R. Marquardt and M. Quack, eds., Molecular Spectroscopy and Quantum Dynamics, Elsevier, Amsterdam, **2021**.
[4] M. Quack, Molecular femtosecond quantum dynamics between less than yoctoseconds and more than days: Experiment and theory, chapter 27 in 'Femtosecond Chemistry', J. Manz, L. Woeste eds. VCH publishers, Weinheim **1995**, *pp* 781-818.
[5] M. Quack, *Chimia*, **2001**, *55*, 753-758 and *Chimia*, **2003**, *57*, 147-160.
[6] A. Kushnarenko, E.Miloglyadov, M. Quack, G.Seyfang,*PCCP*, **2018**, *20*, 10949-10959.
[7] K. v. Puttkamer, M. Quack, *Chimia*, **1985**, *39*, 358-360 and *Chem.Phys.* **1989**, *139*, 31-53.
[8] M. Quack and M Suhm, *J. Chem.Phys.* **1991**, *95*, 28-59.
[9] M. Hippler, L. Oeltjen, M. Quack, *J. Phys. Chem.A,* **2007**, *111*, 12659-12668 and to be published.
[10] C. Manca, M. Quack, M. Willeke, *Chimia*, **2008**, *62*, 235-239.
[11] B. Fehrensen, D.Luckhaus, M. Quack, *Chem. Phys. Lett*, **1999**, *300*, 312-320, and *Chem. Phys.* **2007**, *338*, 90-105.
[12] C.Fabri, R. Marquardt, A. Csaszar, M. Quack, *J.Chem. Phys*, **2019**, *150*, 014102.
[13] M. Quack, *Bunsen-Magazin,* **2022**, *24*, 238-246.
[14] M. Quack, J. Stohner, *Phys.Rev.Lett.* **2000**, *84*, 3807-3810.
[15] M. Quack, G. Seyfang, G. Wichmann, *Adv.Quantum Chem.Phys.* **2020**, *81*, 51-104 and Chem. Science **2022**, *13*, 10598-10643.
[16] G.Wichmann, G.Seyfang, M. Quack, Mol. Phys. **2021**, *119*, e1959073.
[17] M. Quack, Helv.Chim. Acta **2023**, *106*, e202200174