Title	**Molecules and quantum pure states: statistical models of dynamics and thermodynamics at the nanoscale**
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Project description:
The control over the preparation and the time evolution of quantum pure states (wave-functions) became a central challenge in recent years because of the growing interest in the emergence of novel technologies enabled by the quantum nature of matter. Beyond future potential applications, monitoring quantum evolution of small isolated system and single molecule offered an unprecedented view on fundamental aspects as the nature of equilibrium and thermodynamics at the nanoscale and the effect of structured environment on coherent and incoherent quantum dynamics. Most of the current understanding of these issues is based on mixed states as opposed to pure states. The PI and Barbara Fresch, who will collaborate to the project development, have developed original statistical tools for the treatment of quantum pure states evolving according to the Schroedinger equation.[1-4] The PhD project will push forward these investigations, by developing models for the statistical characterization of quantum pure states to provide a thermodynamically-grounded description of both equilibrium properties and quantum dynamics of a probe molecule whose states are controlled by the interactions with the environment. These general methods will be employed for the interpretation of spectroscopic observations and for the characterization of molecules as quantum systems whose properties can be tailored for specific applications in molecular logic and sensing.[5,6] The proposed research will allow the candidate to develop a deep understanding of quantum dynamics and to contribute to the growing scientific effort in envisioning quantum technologies with a special emphasis on the role of molecular systems.

Publications:
[1]B. Fresch, G.J. Moro, Beyond quantum microcanonical statistics, *J. Chem. Phys*. 134 (2011) 05451. [2]B. Fresch, G.J. Moro, Typical response of quantum pure states, *Eur. Phys. J.* B 86 (2013) 233-246. [3]F. Avanzini, B. Fresch, G.J. Moro, Pilot-wave quantum theory with a single Bohm's trajectory, *Found. of Phys.* 46 (2016) 575-605. [4]M. Coden, B. Fresch, G.J. Moro, Quantum Statistical Ensemble Resilient to Thermalization, *J. Phys. Chem. A* 120 (2016) 5074-5082. [5] B. Fresch, D. Hiluf, E. Collini, R. D. Levine, F. Remacle, Molecular decision trees realized by ultrafast electronic spectroscopy. *Proc. Natl. Acad. Sci. U.S.A.* 110, (2013) 17183-17188. [6] B. Fresch, J. Bocquel, S. Rogge, R. D. Levine, F. Remacle, A Probabilistic Finite State Logic Machine Realized Experimentally on a Single Dopant Atom. *Nano Letters* 17 (2017), 1846.

Collaborations/Network: Prof. Francoise Remacle-University of Liege (Belgium). Prof. Raphael D. Levine-The Hebrew University of Jerusalem (Israel). Prof. Sven Rogge (Centre for Quantum Computation and Communication Technology, The University of New South Wales, Australia)**.**

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