Georg Lefkidis, J Nanomed Nanotechnol 2014, 5:5
http://dx.doi.org/10.4172/2157-7439.S1.017

OMICS Group Conferences
Accelerating Scientific Discovery

4th International Conference on
Nanotek & Expo

December 01-03, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

Quantum thermodynamic aspects of magnetic molecules

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In this talk, the author will revise the recent understanding of thermodynamic aspects during functionalization of magnetic molecules. Ever since the laser-induced ultrafast demagnetization of ferromagnetic materials was discovered, spintronics has become a main research field in the area of magnetism and optical control. At the same time the new field of quantum thermodynamics has been emerging studying the effects of the quantum nature of matter on the caloric content of the thermodynamic cycles. However, most of the rules derived in this context stem from investigating model systems such as potential wells and harmonic oscillators. Here author will go beyond these fundamental, yet simplified considerations, and expand them into covering realistic magnetic molecules. Using high-level *ab initio* quantum chemistry the caloric content of nano-heat engines will be studied. These molecular engines comprise of simple dimers and work as Diesel, Otto and Otto-like engines. In the latter, optical excitations are induced by a laser pulse substitute for one of the heat-exchange points. The efficiency, caloric content and work extraction limits of the engines will be analyzed. Furthermore the importance of the spin degree of freedom and the electronic entanglement will be discussed. Some additional concepts, such as the realization of an isobaric process in a quantum context, the evolution of the population distribution profile, and the role of localized transition matrix elements (leading to quantum spin-Hall and spin-Nernts effects) will also be addressed.

Biography

Georg Lefkidis studied Chemistry at the Aristotle University of Thessaloniki, Greece, where he also got his PhD in the Laboratory of Applied Quantum Chemistry in 2002. In 2003, he joined the Physics Department of the University of Kaiserslautern, Germany, first as a Postdoctoral fellow and, since 2007, he is working as a tenured Senior Researcher/Lecturer. He has published more than 40 peer-reviewed articles and serves as referee for several journals. His main research focuses on magnetism and his interests include second harmonic generation, ultrafast (magneto-) optics, laser induced dynamics and spintronics of nanoclusters, as well as the various degrees of freedom involved in quantum thermodynamic processes.

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