



Departmental Seminar

Department of Chemistry

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Time 15:00

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IR-Induced Chemistry: From Conformational Changes to Bond-Breaking Processes and Energetic Crystals

Infrared-induced chemistry has been a relatively unexplored field of research, though its roots may be traced back to the historical work of Hall and Pimentel (*J. Chem. Phys.*, 38, 1889, 1963) where the relative populations of the two conformers of matrix-isolated nitrous acid could be varied by *in situ* IR broadband irradiation. However, only 34 years later, the subject gained importance, when high-selectivity in controlling the chemical reactions could be achieved by introduction of narrowband IR excitation (Pettersson, et al., *J. Am. Chem. Soc.*, 119, 11715, 1997). Since then, IR-induced chemistry has been developing and, nowadays, it can be used to control the molecular conformation with both high selectivity and efficiency. Furthermore, more recently IR excitation has also been shown to be usable to induce bond breaking / bond forming reactions (Nunes, et al., *J. Am. Chem. Soc.*, 139, 17649, 2017). Our Laboratory has been involved in this type of investigations for more than 20 years, and in this talk I will present a summary of some of our most relevant achievements in the field: (a) efficient control of the molecular conformations, including the generation of rare conformers and dimers; (b) changing molecular structure by exciting remotely located in space antennas; (c) using vibrational excitation to facilitate tunneling reactions, including bond-breaking / bond-forming processes; (d) generation of novel high-energy crystals built from high-energy conformers.



Short Biography

Rui Fausto is professor of Chemistry and Director of the Chemistry Research Centre (CQC) at the University of Coimbra, Portugal. He is the leader of the Research Groups on “Theoretical and Computational Chemistry” and on “Molecular Spectroscopy and Thermodynamics”. His research interests range from spectroscopy and solid-state photochemistry to chemical imaging, chemometrics and theoretical and computational chemistry. He has published over 400 scientific articles and published or edited several books, being the editor-in-chief of the Journal of Molecular Structure and member of the editorial boards of several other scientific journals. Along his career, Rui Fausto has occupied many different positions in the administration of the University of Coimbra, including the presidency of the Chemistry Department and the vice-presidency of the Sciences and Technology Faculty. He was awarded several merit prizes, including the Prize for Excellency in Science, from the Portuguese Ministry of Science and the Portuguese Science Foundation. He is member of the European Academy of Arts, Sciences and Humanities (Paris), of several international scientific societies, and coordinator of the Education Committee of the International Observatory of Human Rights.