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Dynamics of chemical reactions under pressure

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High pressure is a powerful tool to finely and widely change the intermolecular geometries in molecular liquids and crystals. Many molecular systems are known to chemically react under pressure, reversibly or irreversibly. In the last years, much work has been done in our laboratory to understand the mechanisms of pressure-induced reactivity at a microscopic level. Experiments relying on static techniques, particularly vibrational and electronic spectroscopy and X-ray diffraction, in combination with MD simulations, have revealed fundamental aspects of the interplay among structure, anisotropic compressibility, and electronic states in opening specific reactions paths[1,2]. Presently, the experimental and theoretical focus is the time resolution of the reactive processes. Infrared pump-probe experiments on compressed liquid water[3,4], unveiling the behavior of the H-bonded network vibrational dynamics under pressure, have been the introductory work to investigate how density affects the dynamics of more complex and reactive systems. At the same time, the dynamics of ice melting (in ice I_h and ice VI) is under study through the use of ultrafast spectroscopic techniques, which will then be employed to investigate the mechanism of formation of hydrates and of solid-state reactions. [1] M. Citroni et al. *Role of excited electronic states in the high-pressure amorphization of benzene.* Proc. Natl. Acad. Sci. 105, 7658 -7663 (2008). [2] M. Citroni, et al., *Nitromethane Decomposition under High Static Pressure,* J. Phys. Chem. B, 114, 9420-9428 (2010). [3] S. Fanetti et al., *Structure and Dynamics of Low-Density and High-Density Liquid Water at High Pressure* J. Phys. Chem. Lett. 5 , 235–240 (2014). [4] A. Lapini et al. *Pressure Dependence of Hydrogen-Bond Dynamics in Liquid Water Probed by Ultrafast Infrared Spectroscopy,* J. Phys. Chem. Lett. 7, 3579-3584 (2016).