MS50.O06

Structural dynamics of ionic materials mapped by femtosecond x-ray diffraction

T. Elsaesser[1]

[1]*Max-Born-Institut, Berlin, Germany*

Relocation of electronic charge plays a key role for functional processes in condensed-phase molecular materials. X-ray diffraction with a femtosecond time resolution allows for spatially resolving transient atomic arrangements and charge distributions [1]. In particular, time-dependent spatial maps of electron density have been derived from x-ray powder diffraction patterns measured with a 100 fs time resolution. In this talk, new results on electron dynamics in transition metal complexes and on field-driven charge relocations in elementary ionic materials will be presented. Crystals containing a dense array of Fe(II)-tris(bipyridine) complexes and their PF6 counterions display pronounced changes of electron density that occur within the first 100 fs after two photon excitation of a small fraction of the complexes [2]. Electron density maps reveal a transfer of electronic charge from the Fe atoms and - so far unknown - from the PF6 counterions to the bipyridine units. The charge transfer displays pronounced Coulomb-mediated many-body features, affecting approximately 30 complexes around the directly excited one. As a second topic, electron relocations induced by strong external optical fields will be discussed [1,3]. This interaction mechanism allows for generating coherent superpositions of valence and conduction band quantum states and inducing fully reversible charge dynamics. While the materials LiBH4 and NaBH4 display electron relocations from the (BH4)- ions to the neighboring Li+ and Na+ ions, LiH exhibits an electron transfer from Li to H. The latter is a manifestation of electron correlations and in agreement with theoretical calculations.

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Keywords: femtosecond x-ray methods, x-ray powder diffraction, electron density map