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Transient electron density maps of ionic materials from femtosecond x-ray powder diffraction

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X-ray diffraction represents a key method for spatially resolving electron distributions in crystalline materials. So far, electron density maps have been derived from stationary diffraction patterns, providing detailed insight into the equilibrium charge distribution and crystal geometry. Functional processes in condensed matter are frequently connected with nonequilibrium excitations resulting in atomic motions and charge relocations on ultrashort time scales. Transient structures are resolved in space and time by novel x-ray diffraction methods with a femtosecond time resolution, giving access to the driving mechanisms and underlying interactions [1]. In this talk, new results are presented on transient electron distributions of ionic materials mapped with the help of femtosecond x-ray powder diffraction. Experiments are based on a pump-probe approach in which an optical pulse initiates structural dynamics and a hard x-ray pulse from a synchronized laser-driven plasma source is diffracted from the excited powder sample. Such measurements reveal the interplay of lattice and charge motions in the photoexcited prototype material KDP (KH_2PO_4) which occur on distinctly different length scales [2]. As a second topic, electron relocations induced by strong external optical fields will be discussed [3,4]. This interaction mechanism allows for generating coherent superpositions of valence and conduction band quantum states and inducing fully reversible charge dynamics. While the materials LiBH_4 and NaBH_4 display electron relocations from the $(\text{BH}_4)^-$ 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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- [4] V. Juvé et al., *Phys. Rev. Lett.* 111, 217401 (2013)