Watching electrons move in real time

September 21 2010

At its most basic level, understanding chemistry means understanding what electrons are doing. Research published in the *Journal of Chemical Physics* not only maps the movement of electrons in real time but also observes a concerted electron and proton transfer that is quite different from any previously known phase transitions in the model crystal, ammonium sulfate. By extending X-ray powder diffraction into the femtosecond realm, the researchers were able to map the relocation of charges in the ammonium sulfate crystal after they were displaced by photoexcitation.

"Our prototype experiment produces a sort of 'molecular movie' of the atoms in action," says author Michael Woerner of the Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie in Germany. "The time and spatial resolution is now at atomic time and length scales, respectively."

Electron positions were mapped by observing the diffraction of X-ray pulses lasting tens of femtoseconds (quadrillionth of a second). Positions of protons and other nuclei were deduced from the locations of regions of high electron density. Within the crystal, the excited electrons transferred from the sulfate groups to a tight channel within crystal matrix. This channel was stabilized by the transfer of protons from adjacent ammonium groups into the channel. This transfer mechanism had not been previously observed or proposed, and the researchers had expected to see much smaller displacements.

According to Woerner, the technique should be applicable to structural studies of materials ranging from biomolecules to high-temperature superconductors. "We expect that the technique will be applied to many interesting material systems." He says. "In principle, femtosecond X-ray powder diffraction can be applied to any crystalline form of matter. Only the complexity of crystals and the presence of heavy elements, which reduces the penetration depth of X-rays, set some constraints."

More information: The Article, "Concerted electron and proton transfer in ionic crystals mapped by femtosecond x-ray powder diffraction" by Michael Woerner, Flavio Zamponi, Zunaira Ansari, Jens Dreyer, Benjamin Freyer, Mirabelle Premont-Schwarz, and Thomas Elsaesser is published in the *Journal of Chemical Physics*. See: jcp.aip.org/jcpsa6/v133/i6/p064509_s1

Provided by American Institute of Physics