

relationships between the synthesis conditions, the oxidation states of the cations, the crystal symmetries and tilt transitions, the anion ordering and the physical properties.

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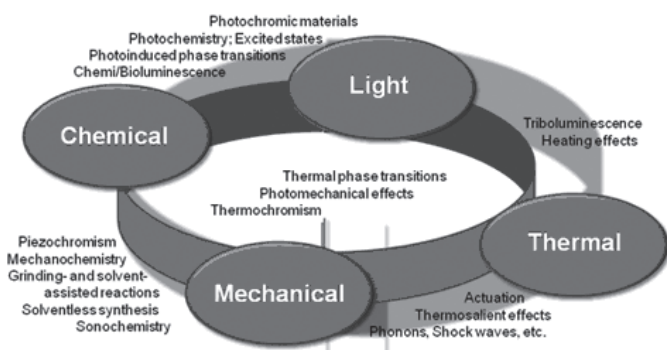
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Molecular mechanisms of photoinduced and thermally induced effects in crystals

Panče Naumov, Department of Material and Life Science, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka (Japan). E-mail: pancenaumov@gmail.com

The recent revival of the interest in solid-state reactivity was partially triggered by the view that it can bridge the ‘classic’ solid-state photochemistry, which has been largely focused on elucidation of mechanisms of photochemical processes in solids, with contemporary chemical fields—notably, materials science and green chemistry—in the course of target-oriented design of photoresponsive/reactive materials. The efforts have been generally aimed at better understanding of structural changes induced by external stimuli (light, temperature and pressure), which can provide a platform for optimization of the performance of new materials for efficient conversion, at a macroscopic scale, among light, chemical, thermal and mechanical energy.



Most attention in the past has been devoted to conversion of *light* into *chemical energy*, and we have contributed to those efforts with a number of case studies that include photodimerizations [1], [2], solid-state rearrangements [3–6], photomagnetization effects and photoinduced phase transitions of persistent organic radicals [7], unstable radical transients [4], [6] exotic radical states [6], as well as photochromic [8–10] and thermochromic systems [11–14]. Recently, however, there has been an increased awareness that the realm of the solid-state research should be expanded to explore processes underlying conversion of light, chemical or thermal energy into *mechanical energy* (work), which has been elegantly exemplified, among the others, by the pioneering works of Boldyreva, Desiraju,

Etter and Toda. The prospects and the practical importance of these processes as solventless routes to synthetically challenging molecular topologies, as energy-storage or actuator materials, or simply as convenient methods for polymorph differentiation, are reflected as increasing number of reports on mechanochemical, piezochromic, sonochemical, triboluminescent and chemiluminescent reactions. By elucidating the molecular mechanism of thermosensitive (jumping) effects [2], [15], photomechanical effects [2] and chemi/bioluminescence [2], [16], [17], we have recently added up a few interesting cases to these, still rare but rapidly expanding studies.

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Insights into reactions of functional materials using pair distribution function analysis

Karena W. Chapman, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, (USA). E-mail: chapmank@aps.anl.gov

Understanding how materials react, at an atomic scale, is key to controlling their functional behaviors. These functionalities can be directly derived from the material’s reactivity, for example, reversible electrochemical reactions for lithium-ion batteries or reactions for sequestering radiological waste. Further, functional properties can be strongly dependent on the structure and morphology produced during synthesis, for example, the catalytic activity of metal nanoparticles.

The structural characterization of these reactions can be challenging, due to the diverse phenomena possible; with multiple components of evolving particle size, morphology, and microstructure from multi-atom clusters to multi-million atom crystals. The pair distribution function (PDF) method shows great promise for providing quantitative insight into the kinetics and structure mechanism of such reactions. Recent advances in experimental methods, have improved the efficiency of X-ray PDF measurements, to allow time-resolved experiments with sufficient resolution to study reactions in solid materials (up to 30 Hz). The PDF analysis probes the complete reaction from clusters to bulk, amorphous or crystalline, liquid or solid. This is in contrast to Bragg crystallographic analysis which is “blind” to the clusters which nucleate before growing into long-range ordered, crystalline materials. The structural insights from the PDF data are obtained in parallel with phase fractions and concentration to allow different components to be distinguished and a robust quantitative analysis.

Keywords: PDF, in-situ, reaction