

MRSEC SEMINAR SERIES

“Snapshots of a Solid State Transformation: Coexistence of Three Phases Trapped in One Single-Crystal.”

Single-crystal-to-single-crystal (SCSC) transformations are crucial in understanding solid-state processes, since they may be studied in detail by single crystal X-ray diffraction (SCXRD). As in molecular chemistry, describing the mechanism and intermediates in those processes is much more challenging. In fact, solid-state intermediates have never been observed to sufficient detail. We have investigated the SCSC process of guest extrusion from a non-porous molecular material, which occurs through ordered diffusion of acetone, with dramatic structural changes.

Its slow kinetics allows thermally trapping the system at various intermediate stages and studying them through SCXRD, offering a window upon the mechanism at the molecular scale. These experiments have unveiled an ordered intermediate phase, radically distinct from the initial and final states, coexisting with them during the process. The full description of an intermediate ordered state in a molecular solid-state transformation is unprecedented and will help to understand the reaction pathways underlying these transformations.



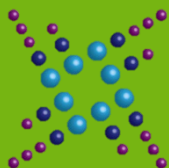
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Tech LR5

4:00 – 5:00 p.m.



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