MS26- Aperiodic and modulated structures

Chairs: Prof. Sven Lidin, Prof. Alla Arakcheeva

MS26-P01

Polarisation via local ordering mechanisms

Emma Wolpert[1], Alistair Overy[1], Peter Thygesen[1], Arkadiy Simonov[1], Mark Senn[2], Andrew Goodwin [1]

1. Department of Chemistry, University of Oxford, Oxford, United Kingdom
2. Department of Chemistry, University of Warwick, Coventry, United Kingdom

email: emma.wolpert@chem.ox.ac.uk

Systems containing correlated disorder are becoming more and more prevalent in materials science.[1] Thus understanding and exploring the disorder-property relationship is becoming of greater importance. In our work[2] we focussed on how aperiodic systems could lead to a macroscopic polarisation. Using classical Monte Carlo simulations, we study a simple statistical mechanical model from local displacements on the square and cubic lattices. Our model contains two key ingredients: a Kitaev-like orientation-dependent interaction between nearest neighbours, and a steric term that acts between next-nearest neighbours. Taken by themselves, each of these two ingredients drives its own form of local ordering to a non-polar disordered phase with a manifold of degenerate ground states. These phases are incapable of driving long-range symmetry breaking, despite the presence of a broad feature in the corresponding heat capacity functions. Instead each ingredient results in a "hidden" transition on cooling to two distinct types of local order. Remarkably, their intersection i.e. the ground state when both interaction contributions are invoked leads to a disordered, but polar, phase which has conceptual parallels to tetragonal $BaTiO_3$ or $KNbO_3$.[3] These key ingredients could potentially be utilised in future material design

References:

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MS26-P02

Polymorphism of $NiSeO_3(H_2O)$ studied on multiphase crystals

Morgane Poupon[1], Nicolas Barrier[2], Olivier Perez[2], Michal Dušek[1], Václav Petříček[1]

1. Department of Structure Analysis Fyzikální Ústav AV ČR, v. v. i, Prague, Czech Republic
2. CRISMAT Laboratory, CAEN, France

email: poupon@fzu.cz

Inorganic materials with a layered structure are interesting for their potential exchange and/or storage properties [1]. These structures typically have weak intermolecular bonds between their different layers, like Van der Waals or hydrogen bonds [2]. However, weak bonds may lead to stacking faults or the intergrowth of phases inside the crystal. These defects could induce diffuse scattering and additional reflections, which can be observed on the reciprocal planes reconstructed from X-ray single crystal measurement. Understanding this complex order can allow us to solve structures of metastable polymorphs and to apprehend the processes of transformation towards their stable states. The family of lamellar compounds MSeO3(H2O) (M = Mn, Co, Ni, Zn, Cd) [3] is of interest regarding their several polymorphs. The cohesion of these structures is provided by hydrogen bonds. The NiSeO3(H2O) crystals were synthesized using hydrothermal synthesis under low-pressure and low temperature conditions.
We will present how the formalism of (3 + 1)d superspace can help to reveal the crucial role of weak interaction and the existence of intergrowth between two polymorphs in the crystal. Then, we will present the temperature stability study using low and high-temperature single crystal X-ray diffraction measurements of these multiphase crystals.
References:

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