

= 0 to 0.2 has been prepared and the evolution of the crystal structures studied using high-resolution powder X-ray and neutron diffraction. The amount of the Jahn-Teller active Mn^{3+} ions is controlled by partially replacing the Mn with Cr. At room temperature samples with $x \leq 0.05$ only display out of phase rotations of the octahedral along c -axis leading to tetragonal $I4/mcm$ space group symmetry. Progressively replacing the Mn^{3+} with Cr^{3+} triggers additional rotations of the corner sharing octahedra ($a^-b^+a^-$ tilt system) such that samples with $x \geq 0.10$, adopt orthorhombic $GdFeO_3$ -type structure in space group $Pbnm$. The lowering of symmetry upon addition of Cr is in response to the decrease in the effective size of the B -type cation ($B = Mn$ and Cr). Equally importantly the Cr^{3+} acts to remove the Jahn-Teller type distortions induced by the presence of Mn^{3+} . High temperature diffraction measurements show that the increasing of the tilts through the addition of Cr in $Ca_{0.4}Sr_{0.4}Nd_{0.2}Mn_{1-x}Cr_xO_3$ stabilizes an orthorhombic structure and a more complex sequence of phase transition is observed, namely $Pbnm \leftrightarrow I4/mcm \leftrightarrow Pm\bar{3}m$.

Keywords: phase transition, perovskites, high_resolution_powder_diffraction

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Evolutionary crystal structure prediction: method and results

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While most of the known materials have been discovered through experiments, one wonders if theory will ever become capable of leading materials discovery. The evolutionary methodology USPEX [1] has been a major step towards this goal as it provides, given just the chemical composition and pressure/temperature conditions, the stable structure and a set of low-energy metastable structures. Important developments of this method were made thanks to the theory of energy landscapes [2].

Some of the applications are:

1. New stable high-pressure phase of boron, γ -B [3]. This superhard phase shows a surprising degree of charge transfer between boron sites, which affects many physical properties [3].
2. Transparent insulating phase of sodium [4] and new phases of calcium [5], $CaLi_2$ [6], nitrogen [7].
3. Unusual high-pressure behavior of methane CH_4 , silane SiH_4 [8], germane GeH_4 [9] and stannane SnH_4 [10].

Many methodological developments happened recently. The method has been extended to molecular crystals, nanoparticles, and crystalline surfaces. It can now deal with systems with up to several hundred atoms in the unit cell. Its extension to variable-composition systems allows simultaneous finding of stable chemical compositions and the corresponding crystal structures in a multinary A-B-C... system. It is now also possible to optimize the structure and chemical composition with respect to a given physical property [11]. I will discuss newly predicted carbon allotropes with special properties.

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In silico crystallisations of organic molecules: what have we learnt?

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Since 1999, the blind tests for crystal structure prediction (CSP) have motivated the regular development and testing of CSP methodologies for small organic molecules. Blind tests' participants are sent the chemical diagrams of the target molecules and the experimental crystal structures are withheld until participants have submitted their predictions (three submissions per target). These communal experiments, organised regularly at the Cambridge Crystallographic Data Centre (CCDC), have recorded and tracked numerous challenges and successes over the years (1999 [1], 2001 [2], 2004 [3], 2007 [4] and 2010).

This talk will present the results of the 2010 blind test for CSP in which 15 research groups participated. Six different targets were attempted for prediction, three of which had a similar complexity to targets in previous blind tests: two small rigid molecules and one small flexible molecule. In addition to these, the 2010 blind test participants were challenged with the prediction of a 1:1 molecular salt, a highly flexible molecule and a polymorphic hydrate. The knowledge acquired over previous blind tests as well as the challenges faced in the present one will be discussed. Although there was no single method successful in all categories, every target had at least one successful prediction.

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Keywords: prediction, crystal, computation