Challenging Chemical Intuition: Pressure-induced Abnormal Phase Transition

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bnormal Phase Transition

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High pressure technique is one of the most important methods to discover materials with exotic properties since it can synthesize new phases that can be recovered as metastable phases at ambient. The interior of all planets are ubiquity within ultra-high pressure. Thus, research on the properties under pressures is essential to enrich our knowledge of the mystic universe.

Perovskite structure is the most common prototype form for functional materials, while also the main constituent of the Earth Mantle. Consequently, studies of pressure correlated perovskite structures are of great significance.

Prof. JIN Changqing's team from Institute of Physics of the Chinese Academy of Sciences (CAS) has worked on perovskite-like new materials by using high pressure synthesis for long time. With advanced new highpressure techniques, they designed and successfully fabricated a serial of new functional materials with perovskite-like structures.

Order disorder effects in materials are of fundamental interest to solid state sciences. Polymorphs with identical chemical formula, but different ordering degrees, can alter crystal symmetry dramatically and hence modify properties-like stability, magnetism,

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Reference

A Pressure-Induced Inverse Order–Disorder Transition in Double Perovskites
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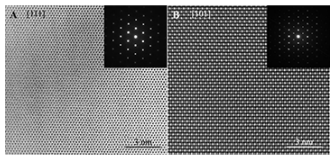

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thermo-and electrical transport, elasticity, etc. Usually order disorder transitions are controlled by temperature or compositions.

In addition, pressure has also been applied to modify atomic ordering with remarkable efficiency, thanks to the advancement of high pressure techniques.

Very recently, Prof. JIN's team made important progress on new type of perovskite compounds, namely the double perovskites $A_2B'B''O_6$, which was synthesized under extremely high-pressures.

For most of known materials, pressure tends to increase number of coordination, and hence make a structure ordered. Chemical intuition indicates that the disordered phases will have larger lattice volumes since the distance of neighboring B''-B'' will be additionally enlarged owing to strong Coulomb repulsion.

As a result, B-site disordered cannot be stabilized under highpressures. Previous reports indeed confirmed that pressure always increase B-site ordering.

Associate professor DENG Zheng, Dr. LI Wenmin and Dr. ZHAO Jianfa from Prof. JIN's team synthesized a new B-sited ordered double perovskite Y_2CoIrO_6, and further discovered pressure-induced B-site disordering phenomena.

With increasing synthesis pressures, the material showed B-sited order (at 0 GPa), partial order (at 6 GPa) and complete disorder (at 15 GPa). It is interesting that 15 GPa corresponds to the pressure around boundary region between upper Mantle and lower Mantle wherein many perovskite materials form.

Along with the transition from ordered structure to disordered one, the magnetic property changes from long-range ferrimangenet to short-range spin-glass-like state. The origin of the pressure induced inverse order disorder transition is that the disordered phase has smaller unit cell volume due to the unique combination of B'-O and B''-O bond strength, namely orbital hybridizations. The physical mechanism is supported by the theory calculations based on built-up of thermo-statistical model.

The study is published on *Angewandte Chemie-International Edition (https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202001922)* as cover-page paper and hot paper. The discovery of counter chemical intuition will lead to reconsideration of the effects of pressures in solid state sciences, as highlighted in the coverpage guideline of *Angewandte Chemie-International*.

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Recently, researchers led by Dr. WANG Yumei from Institute of Physics, teaming up with other scientists from home and abroad, identified the relation between the asymmetry and materials' parameters, which can be used to predict the performance of unreported type of a give...

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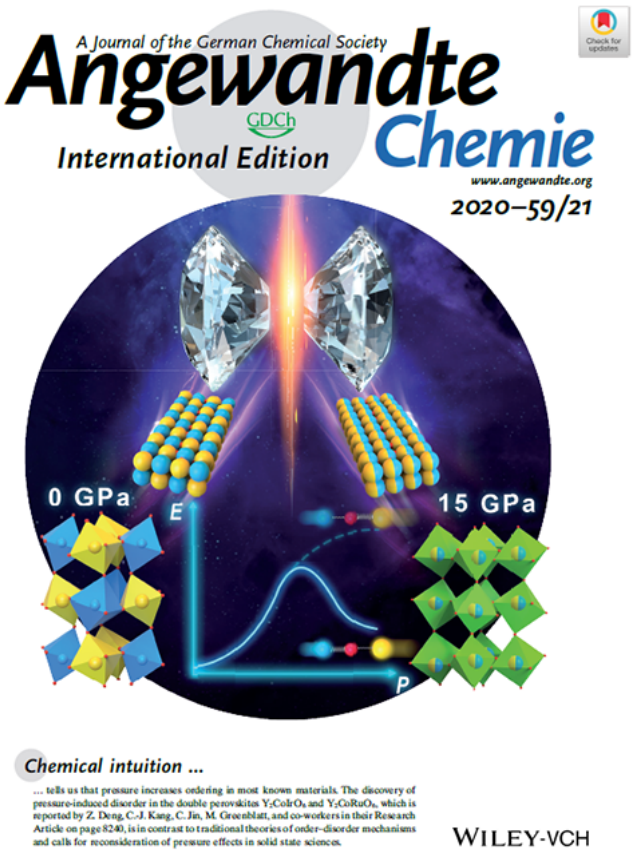

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