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Challenging Chemical Intuition: Pressure-induced Abnormal Phase Transition

Editor: ZHANG Nannan | May 26, 2020

Abnormal 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,

Contact

JIN Changqing

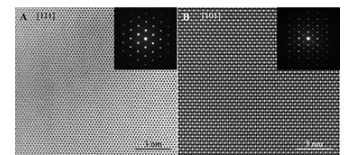
Institute of Physics

[\(http://english.iop.cas.cn/\)](http://english.iop.cas.cn/)E-mail: jin@iphy.ac.cn<mailto:jin@iphy.ac.cn>

Reference

A Pressure-Induced Inverse Order-Disorder Transition in Double Perovskites
<https://onlinelibrary.wiley.com/doi>

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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 ferrimagnet 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*.

The study is supported by the Ministry of Science and Technology, the National Natural Science Foundation of China, and the Youth Innovation Promotion Association of CAS.

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...



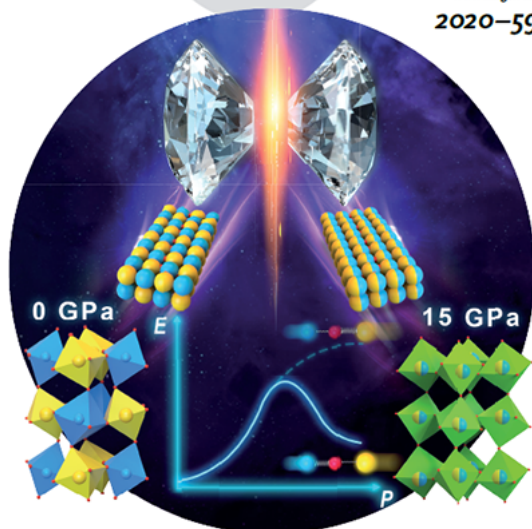
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Chinese Scientists Unlock Structural Secrets of Whale Baleen

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Nov 21, 2018

Chinese scientists working with other researchers have for the first time uncovered the underlying mechanisms of the hierarchical structure of baleen, with an eye toward developing advanced engineered materials. The study shows that the nanoscale structure of baleen's in...



Chemical intuition ...

... tells us that pressure increases ordering in most known materials. The discovery of pressure-induced disorder in the double perovskites Y_2CoIrO_6 and Y_2CoRuO_6 , which is reported by Z. Deng, C.-J. Kang, C. Jin, M. Groenblatt, and co-workers in their Research Article on page 8240, is in contrast to traditional theories of order-disorder mechanisms and calls for reconsideration of pressure effects in solid state sciences.

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Cover page story of *Angewandte Chemie* for this work (Image by JIN Changqing)

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CONTACT US



86-10-68597521 (day)

86-10-68597289 (night)



86-10-68511095 (day)

86-10-68512458 (night)



cas_en@cas.cn



52 Sanlihe Rd., Beijing,
China (100864)

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