

Microsymposium

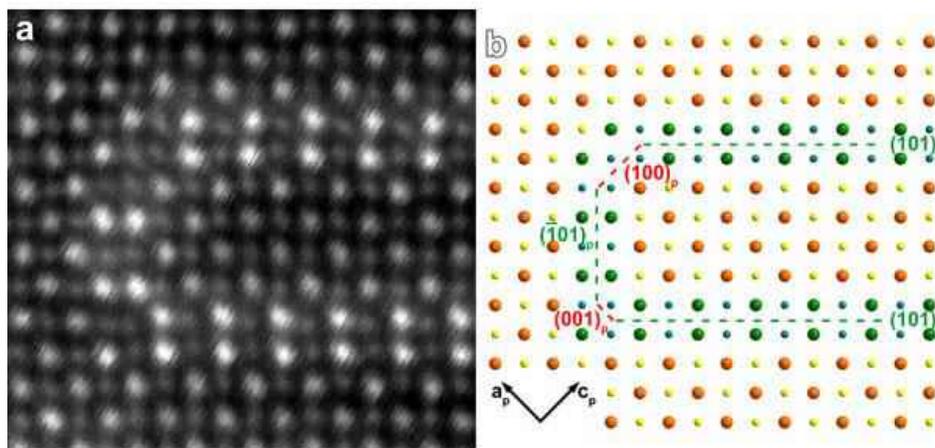
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New modular oxide structures using lone pair cations as “chemical scissors”

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It is known that lone pair cations, such as Bi³⁺ or Pb²⁺ have a flexible coordination environment that enables them to operate as “chemical scissors”. Their flexibility reduces the strain that would otherwise be present at the interfaces separating structure modules. We have found that in complex oxides it allows many variants of interfaces, for example crystallographic shear planes or (non)conservative twin planes in structures, enabling the synthesis of new structural families. A common characteristic for all these new compounds is the presence of magnetical frustration. As a first example, this concept allowed to introduce crystallographic shear planes into the perovskite structure, a feat that was considered highly unlikely before. This allowed to generate a new anion deficient perovskite based homologous series $AnBnO_{3n-2}$ ($n = 4 - 6$). There is magnetic frustration at the crystallographic shear plane separating the perovskite blocks, due to competing FM and AFM interactions. Also incommensurately modulated perovskites can be obtained, for example $(Pb,Bi)_{1-x}Fe_1+xO_{3-y}$. These arise by replacing Bi³⁺ with Pb²⁺, which introduces an oxygen deficiency, which is then accommodated by periodically spaced CS planes to reduce the coordination of the A-cations at the interface. The flexible coordination environment of Bi³⁺ and Pb²⁺ makes them ideally suited for these A cation positions. Other possibilities were encountered in BiMnFe₂O₆ and Bi₄Fe₅O₁₃F. In BiMnFe₂O₆ the Bi³⁺ induces the existence of a non-conservative twin plane. The result is a new structure type with hcp structured modules. In Bi₄Fe₅O₁₃F, the Bi³⁺-cations separate layers with magnetically frustrated Cairo lattices.



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