Computer Predictions on Hybrid Organic-Inorganic Perovskites

Hybrid or metal organic framework (MOF) perovskites of general composition, ABX₃, are known to show interesting properties which can lead to a variety of technological applications. Our first principles study shows they are also potential candidates for exhibiting cooperative spin-state transitions upon application of external stimuli,[1] and two-dimensional magnetism.[2,3] We also predict new hybrid double perovskites with B-site cation ordering. [4]

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