

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Relevance of Jahn-Teller effect in strongly anisotropic metal sites

NAOYA IWAHARA, VIERU VEACHESLAV, LIVIU UNGUR, LIVIU CHIBOTARU, Katholieke Universiteit Leuven — Recently, heavy transition metal compounds have been intensively investigated because of their unusual magnetic properties driven by strong spin-orbit coupling. In particular, the systems with highly degenerate local electronic states, as represented by the d^1 double perovskites containing Mo^{5+} , Re^{6+} , Os^{7+} , show enhanced anisotropy in exchange interactions. Despite the four-fold (quasi) degeneracy in the d^1 materials, the Jahn-Teller (JT) distortion has not been observed in many of them by x-ray and neutron diffraction down to a few Kelvin. This “violation” of JT theorem has been often reported, whereas no explanation for it has been given so far. Here, we address the nature of the JT effect in cubic double perovskites with *ab initio* based methodology. We calculated the local properties such as crystal field levels, vibronic coupling, and magnetic moments, by using state-of-the-art post Hartree-Fock method. The JT stabilization for these ions is obtained weak to intermediate compared to the frequency of the local active vibration. This implies either the absence or a dynamical character of JT effect, explaining the absence of static JT distortions. The influence of the dynamical JT effect on local magnetic properties will be presented.

Naoya Iwahara
Katholieke Universiteit Leuven

Date submitted: 18 Nov 2016

Electronic form version 1.4