Vibronic order and emergent magnetism in cubic d1 double perovskites

Naoya Iwahara¹, Liviu F. Chibotaru²

¹Graduate School of Engineering, Chiba University, Chiba, Japan
²Theory of Nanomaterials Group, KU Leuven, Leuven, Belgium

The synergistic interplay of different interactions in materials leads to the emergence of novel quantum phenomena. Spin-orbit and vibronic couplings usually counteract each other, however, in cubic d¹ double perovskites [Fig. (a)] they coexist and give rise to spin-orbit-lattice entanglement with unquenched dynamic Jahn-Teller effect on the metal sites [1]. The correlation of these entangled states induced by intersite interactions was not assessed so far. Here, we investigate the joint cooperative effect of spin-orbit and vibronic interactions on the formation of the ordered phases in d¹ double perovskites [2]. We developed a microscopic vibronic approach that concomitantly treats the competing spin-orbit and vibronic interactions in cubic d¹ double perovskites. We found that the magnetic order coexists with the vibronic order characterized by ferro/antiferro arrangement of vibronic quadrupole moments on sites. The present theory allows the rationalization of the mechanism of puzzling phases in the 5d¹ double perovskites: the high-temperature quadrupole orders above the magnetic transition of the so called FM110 phase in rhenium compounds [3] and the antiferromagnetic phase with tetragonal compression in tantalum compounds [4] [Fig. (b)].

Figure. (a) Conventional cell of the double perovskites. (b) Vibronic ordered phase diagram and the relation between the ordered states with existing materials.