Vibronic order and emergent magnetism in cubic d1 double perovskites

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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 d^1 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 d^1 double perovskites [2]. We developed a microscopic vibronic approach that concomitantly treats the competing spin-orbit and vibronic interactions in cubic d^1 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 $5d^1$ 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)].

(a) (b)

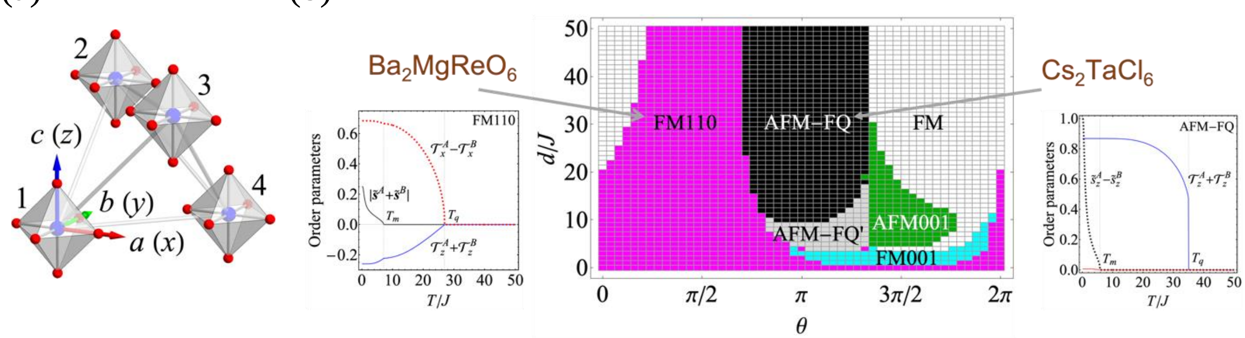

Figure. (a) Conventional cell of the double perovskites. (b) Vibronic ordered phase diagram and the relation between the ordered states with existing materials.

[1] N. Iwahara, V. Vieru, and L. F. Chibotaru, *Phys. Rev. B* **98**, 075138 (2018).
[2] N. Iwahara and L. F. Chibotaru, arXiv:2211.09577
[3] D. Hirai *et al.*, *Phys. Rev. Research* **2**, 022063(R) (2020).
[4] H. Ishikawa *et al.*, *Phys. Rev. B* **100**, 045142 (2019).