Anti-relativistic Jahn-Teller polaron in a spin-orbit entangled oxide

Lorenzo Celiberti^{1,2}, Dario Fiore Mosca¹, Giuseppe Allodi³, Leonid V. Pourovskii^{4,5}, Anna Tassetti², Paola Caterina Forino², Roberto De Renzi⁵, Vesna Mitrović⁶, Erick Garcia⁶, Rong Cong⁶, Patrick Woodward⁷, Samuele Sanna², and Cesare Franchini^{1,2}

¹ University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria

² Department of Physics and Astronomy 'Augusto Righi', Alma Mater Studiorum - Università di Bologna, Bologna, 40127 Italy

³ Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy

⁴ Centre de Physique Théorique, Ecole polytechnique, CNRS, Institut Polytechnique de Paris, 91128 Palaiseau Cedex, France

⁵ Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

⁶ Department of Physics, Brown University, Providence, Rhode Island 02912, USA

⁷ Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio 43210, USA

Polarons are quasiparticles originating from strong electron-phonon interaction in polarizable materials. In Jahn-Teller (JT) active media, distortions arising from symmetry braking might favour or encumber polaron formation and thereby we speak of JT or anti-JT polarons [1]. So far, these quasiparticles have been observed in doped 3d transition metal oxides, as $La_{1-x}Sr_xMnO_3$ and superconductive $La_{2-x}Sr_xCuO_4$ [1, 2]. However, in heavier 5d transition metal oxides, the more delocalised nature of the orbitals is likely to hinder polaron formation and spin-orbit (SOC) effects become important. Their repercussions on the $t \otimes E$ and $t \otimes T$ adiabatic energy surfaces of d electron impurities have been recently studied using model Hamiltonian approaches [3, 4]. Using ab initio calculations and magnetic measurements we show that polarons form in the 5d spin-orbit coupled double perovskite Ba_2NaOsO_6 . In particular, we observe that the quasiparticle stability strongly depends on the competing actions of SOC and a local tetragonal JT distortion. These unique vibro-spin-orbital properties identify a new type of quasiparticle in Ba_2NaOsO_6 that we name anti-relativistic Jahn-Teller polaron.

- [1] C. Franchini, M. Reticcioli, M. Setvin, and U. Diebold, Nature Reviews Materials, 1 (2021).
- [2] G.-m. Zhao, M. B. Hunt, H. Keller, and K. A. Müller, Nature 385, 236 (1997).
- [3] S. V. Streltsov and D. I. Khomskii, Physical Review X 10, 031043 (2020).
- [4] S. V. Streltsov, F. V. Temnikov, K. I. Kugel, and D. I. Khomskii, Physical Review B 105, 205142 (2022).