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Mott Multiferroics and Ferroelectric Metals from Dynamical Mean-Field Theory combined with Density-Functional Theory[1]

MASSIMO CAPONE, International School for Advanced Studies (SISSA) and CNR-IOM, Trieste

Multiferroic materials, in which ferroelectricity and long-range magnetic ordering coexist, are natural candidates for applications. In this perspective, the most promising compounds are those in which the two phenomena do not simply coexist, but they influence each other through a magnetoelectric coupling. We present different applications of Density Functional Theory combined with Dynamical Mean-Field Theory in which electron-electron correlation effects are crucial in the stabilization of multiferroic behavior and in the magnetoelectric coupling. Within this wide family we can distinguish different cases. In $Sr_{0.5}Ba_{0.5}MnO_3$ the multiferroic behavior is associated with a Mott insulating state in which the Mn half-filled t_{2g} orbitals are responsible of the magnetic properties and the value of the polarization is strongly affected by the magnetic state [1]. $LiOsO_3$ shares the same electronic configuration with half-filled Os t_{2g} orbitals. Despite this configuration enhances the effect of electron-electron interactions, the material remains metallic and represents a peculiar ferroelectric metal [2]. We propose however how to turn this non-magnetic polar metal into a multiferroic through the design of a superlattice, which increases the degree of correlation, leading to Mott localization of the Os orbitals [3]. In completely different systems, such as organic crystals like $(TMTTF)_2$-X, strong correlations can lead to multiferroicity in organic crystals such as $(TMTTF)_2$-X, where charge ordering promotes a polarization which is favored by an antiferromagnetic ordering [4]. We finally discuss how strong correlations can play a major role away from half-filling when the Hund's coupling is sizable in compounds with a nominal valence of, e.g., two electrons in the three t_{2g} orbitals. Such "Hund's metals" are correlated despite being far from Mott localization. This physical regime can be a fertile ground to obtain other ferroelectric metals.

[1] G. Giovannetti, S. Kumar, C. Ortix, M. Capone, and J. van den Brink Phys. Rev. Lett. 109, 107601(2012)
[2] G. Giovannetti and M. Capone, Phys. Rev. B 90, 195113 (2014)
[3] G. Giovannetti, D. Puggioni, M. Capone and J. M. Rondinelli, in preparation
[4] G. Giovannetti, S. Kumar, J.-P. Pouget, and M. Capone, Phys. Rev. B 85, 205146 (2012); G. Giovannetti, R. Nourafkan, G. Kotliar and M. Capone, arXiv:1405.1528

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