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Altermagnetism arising from a spontaneous electronic instability

Altermagnetism is attracting great interest as a new third type of collinear magnetic order, distinct by symmetry from conventional ferromagnetism and antiferromagnetism. Now, a mechanism for an interaction-induced formation of altermagnetism in isotropic crystals is presented, based on spontaneous orbital ordering.

Until a few years ago, collinear magnetic order was thought to exist only in two basic forms, namely ferromagnetism or antiferromagnetism. In ferromagnets, all spins on a lattice are aligned in the same direction, giving rise to a nonzero net magnetization. In antiferromagnets, instead, neighbouring spins are antiparallel to each other so that half of the spins point in one direction and the other half in the opposite direction, forming an alternating magnetic pattern with no net magnetization. While in the case of ferromagnetism the net magnetization is accompanied by an energy split of upward and downward spin bands, in the case of antiferromagnetism the spin-up and spin-down energy bands are degenerate, having the same dispersion in momentum space. This so-called Kramers spin degeneracy is a consequence of the upward and downward spin sublattices being connected to one another by a lattice translation operation or inversion symmetry. The lifting of spin degeneracy and a vanishing net magnetization were considered mutually exclusive in collinear magnets, until recent theoretical works[1,2] and an experimental study on MnTe[3] have demonstrated the existence of a third type of collinear magnetic order, called altermagnetism. In this type of magnetic state, neighbouring spins are antiparallel and there is no net magnetization as in antiferromagnets. Yet, the symmetry operation required to connect opposite-spin sublattices involves a lattice rotation, resulting in a nonrelativistic spin splitting of energy bands in momentum space with a sign pattern related to the rotational symmetry. It is worth mentioning that this effect is significantly larger and qualitatively distinct, in terms of symmetry classification, from the spin splitting that may arise from relativistic spin-orbit coupling effects.

In the initial theoretical proposals and experimental demonstration of altermagnetism, the peculiar scenario of opposite-spin sublattices being related by rotations, rather than lattice translations, is realized by searching for materials with crystallographic anisotropies within the unit cell. For example, asymmetric ligands on neighbouring bonds, as shown in the top-left panel of Fig. 1, could provide the required microscopic mechanism. In this situation, an electron density anisotropy is already embedded in the crystal potential, so that the magnetic ordering transition is simply turning the local crystal anisotropy into spatially anisotropic spin-polarized states (bottom-left panel of Fig. 1). Now, writing in *Physical Review Letters*[4], Valentin Leeb and collaborators predict the possibility of realizing altermagnetism in isotropic crystal structures as a spontaneous instability driven by electronic correlations.

In the mechanism envisaged by Leeb et al.[4], an orbital order transition occurring in a minimal model for transition-metal systems, with directional d_{xz} and d_{yz} orbitals, provides the required spontaneous sublattice anisotropy. This transition, in combination with an antiferromagnetic exchange interaction, gives rise to a d-wave altermagnetic phase, where opposite-spin sublattices and spin-polarized bands are related by a 90° rotation (bottom-right panel of Fig. 1). "The study of altermagnets was focused on crystal symmetry groups, e.g. those where the crystal structure leads to non-trivial sublattices related by rotations. Having worked on iron-based superconductors I knew that electronic correlations could lower the crystal symmetry spontaneously via orbital ordering phase transitions," comments Johannes Knolle, the supervisor of this project. "For iron-based superconductor parent compounds both the magnetism and orbital ordering are of the wrong type to give altermagnetism. However, in this current project together with PhD student Valentin Leeb, we realised that a staggered orbital ordering together with conventional Néel antiferromagnetism indeed does give rise to a spontaneous altermagnet."

An exciting outcome of these findings is that "it widens considerably the range of possible [altermagnetic] materials because, at the moment, the focus is on crystals with low symmetry and our mechanism could also give altermagnetism in high symmetry crystals," explains Knolle. In this context, while the identification of materials with staggered orbital order coexisting with Néel antiferromagnetism can be challenging, a promising

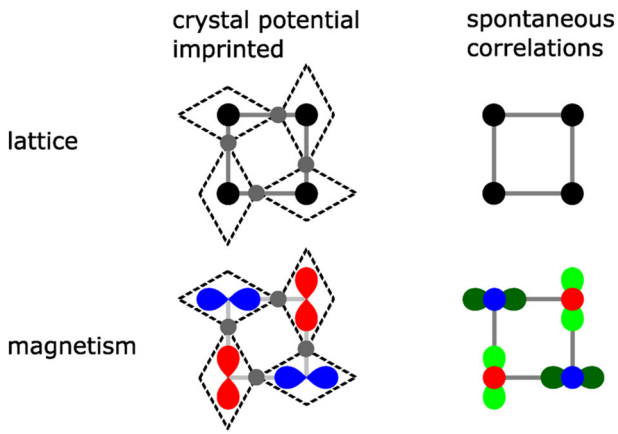

Fig. 1 | Different microscopic mechanisms for altermagnetism. In the left column, the crystal potential is already anisotropic within the lattice unit cell. When a magnetic transition occurs, spin-polarized states appear on the red and blue sublattices. In contrast to standard antiferromagnetism, the symmetry connecting the two sublattices involves a spin-flip operation combined with a 90° rotation (instead of a lattice translation). In the right column, the crystal potential is fully isotropic. However, electron correlations give rise to a spontaneous staggered orbital order (light and dark green electronic states) which provides the required local anisotropy for altermagnetic order (red and blue spin states). Figure reused with permission from Leeb et al.[4], © 2024 by the American Physical Society, https://doi.org/10.1103/PhysRevLett.132.236701.

direction in terms of candidate materials is offered by cubic vanadates[5], where such a coexistence has been experimentally demonstrated. In addition to expanding the range of candidate altermagnets, the current interaction-based mechanism "may turn out to be useful for 'switching altermagnetism' on/off", an important aspect for potential spintronic applications, "or maybe magneto-electric effects could be used for more efficient coupling via the orbital degrees of freedom," concludes Knolle.

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