2D altermagnets from high throughput computational screening: symmetry requirements, chiral magnons and spin-orbit effects

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We present a high throughput computational search for altermagnetism in two-dimensional (2D) materials based on the Computational 2D Materials Database (C2DB). We start by showing that the symmetry require- ments for altermagnetism in 2D are somewhat more strict compared to bulk materials and applying these yields a total of 7 altermagnets in the C2DB. The collinear ground state in these monolayers are verified by spin spiral calculations using the generalized Bloch theorem. We focus on four *d*-wave altermagnetic materials belonging to the $P2'_1/c'$ magnetic space group - RuF_4, VF_4, AgF_2 and OsF_4. The first three of these are known experimen- tally as van der Waals bonded bulk materials and are likely to be exfoliable from their bulk parent compounds. We perform a detailed analysis of the electronic structure and non-relativistic spin splitting in *k*-space exempli- fied by RuF_4. The magnon spectrum of RuF_4 is calculated from the magnetic force theorem and it is shown that the symmetries that enforce degenerate magnon bands in anti-ferromagnets are absent in altermagnets and give rise to the obtained non-degenerate magnon spectrum. We then include spin-orbit effects and show that these will dominate the splitting ofmagnons in RuF_4. Finally, we provide an example of *i*-wave altermagnetism in the 2H phase of $FeBr_3$.

Figures

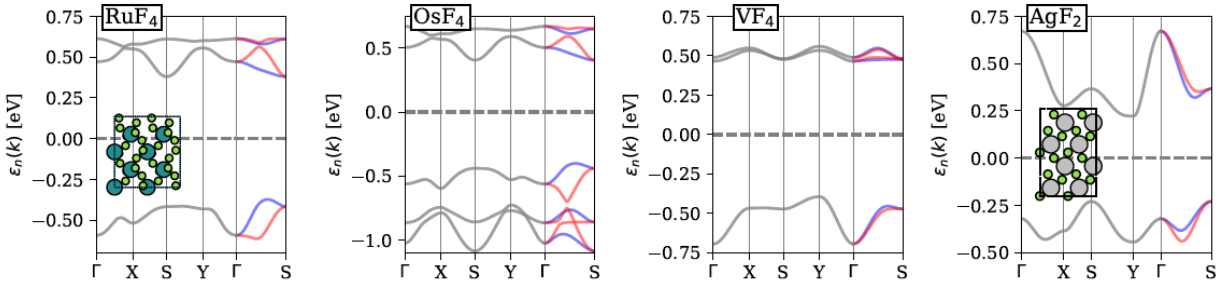

Figure 1: The band structures of altermagnetic RuF4, OsF_4, VF_4 and AgF_2 calculated without SOC. The blue and red lines correspond to the two spin channels. The insets show the atomic structures in 2x2 supercells (OsF_4 and VF_4 are isostructural to RuF_4).

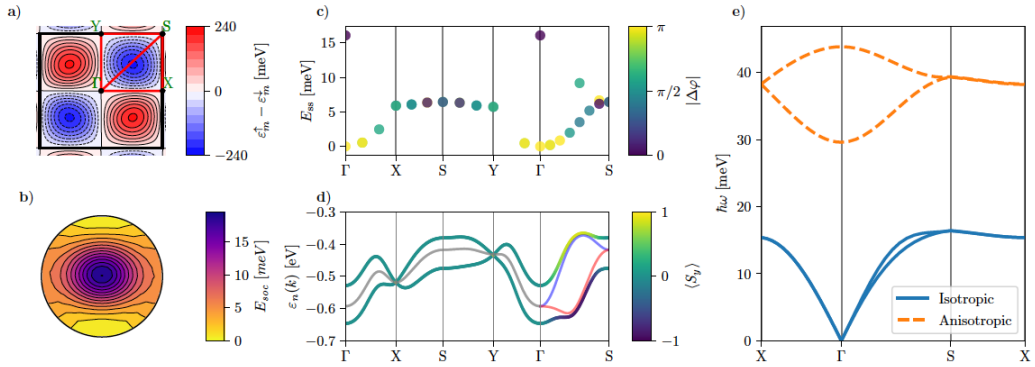

Figure 2: Electronic and magnetic properties of altermagnetic RuF_4. a) The spin splitting of the two highest occupied bands calculated without SOC. b) The spin-orbit energy as a function of spin orientation on the upper hemisphere shown as a stereographic projection. c) Spin spiral dispersion of RuF_4 coloured by the angle between the two magnetic moments in the unit cell. d) The electronic band structure with and without SOC. The bands including SOC are coloured according to ⟨Sy⟩ in units of h/2. e) Magnon dispersion excluding (isotropic) and including (anisotropic) SOC