Highlights

Activity C - Innovative materials with strong interplay of spin, orbital, charge and topological degrees of freedom - 2021

Half-metallic ferromagnetism in layered CdOHCl induced by hole doping

H. Banerjee[1,3], P. Barone[2], S. Picozzi[2]

[1]The Abdus Salam International Centre for Theoretical Physics (ICTP), 34151 Trieste, Italy
[2]CNR-SPIN, UOS Aquila c/o Università G. d'Annunzio, Via dei Vestini 31, 66100 Chieti, Italy
[3]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz 8010, Austria

2D Materials **8**, 025027 (2021)

Next-generation spintronic devices will benefit from low-dimensionality, ferromagnetism, and half–metallicity, possibly controlled by electric fields. These technologically–appealing features are predicted, via first-principles calculations, to be combined in doped CdOHCl, a van der Waals material from which 2D layers may be exfoliated. A homogeneous hole–doping is found to give rise to p-band itinerant magnetism in both the bulk and few-layer phases arising from a Stoner instability: as the Fermi level is tuned via hole–doping through singularities in the 2D-like density of states, ferromagnetism develops with large saturation magnetization of 1 μ_B per hole, leading to a half-metallic behaviour for layer carrier densities of the order of 10^{14} cm^{-2} . Furthermore, we put forward electrostatic doping as an additional handle to induce magnetism in monolayers and bilayers of CdOHCl. Upon application of critical electric fields perpendicular to atomically–thin-films (as low as 0.2 and 0.5 V $Å^{-1}$ in the bilayer and monolayer case, respectively), we envisage the emergence of a magnetic half-metallic state.

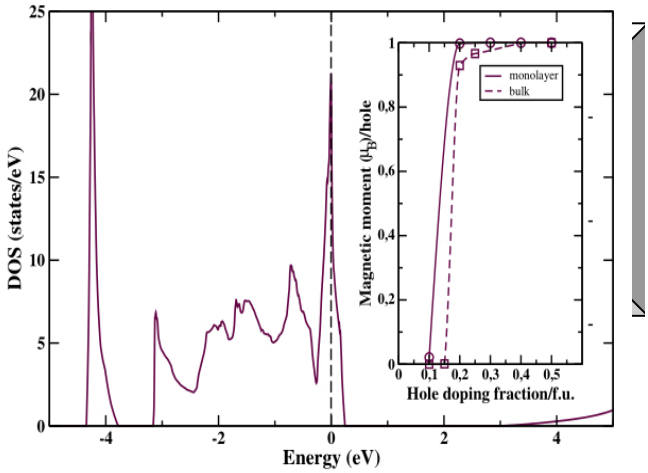

Fig. 1: Total density of states in the paramagnetic phase at the critical hole doping, tuning the Fermi energy at a sharp peak in the DOS and driving a Stoner-like magnetic instability. CdOHCl displays a half-metallic ferromagnetic phase in both bulk and monolayer structures, with a magnetic moment quickly saturating to 1 μ_B per hole as a function of the hole concentration, as shown in the inset.

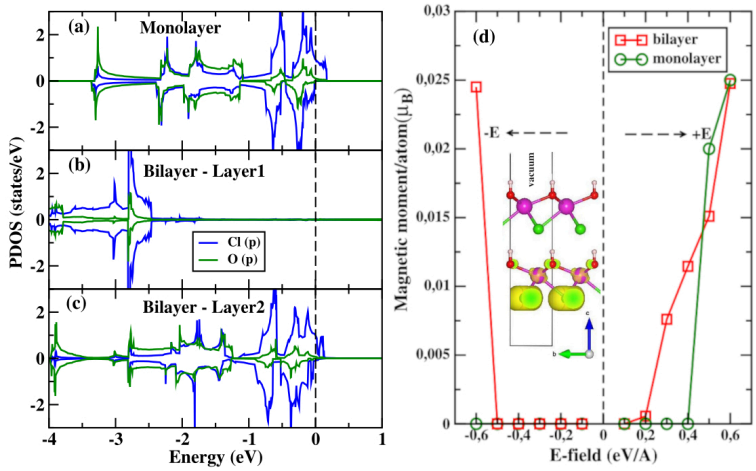

Fig. 2: Projected DOS for monolayer (a) and bilayer (panels (b),(c) for top and bottom layers) on application of an electric field E=0.6 eV $Å^{-1}$, highlighting field-induced band shift and fully spin-polarized half-metallicity. Panel (d) shows the magnetic moments as a function of applied electric fields: the asymmetric response as well as the stronger tendency of bilayer to develop magnetism are ascribed to the inherent polarity of CdOHCl atomic stack (displayed in the inset, alongside the magnetic density of