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Piezomagnetic response in $CrPS_4$ monolayer

We performed first-principles calculations to investigate the magnetic, mechanical and electronic properties of the tetrachalcogenide $CrPS_4$. Although bulk $CrPS_4$ has been shown to exhibit a low-dimensional antiferromagnetic (AFM) ground state where ferromagnetic (FM) Cr-chains are coupled antiferromagnetically, our calculations indicated that the monolayer can be transformed to an FM material by applying a uniaxial tensile strain of ⍰4% along the FM Cr-chain direction. The AFM-to-FM transition is explained to be driven by an increase of the exchange interaction induced by a decrease in the distance between the FM Cr-chains. A huge nonlinear piezomagnetism was predicted at the strain-induced magnetic phase boundary. Our study provides insight about rational design of single-layer magnetic materials for a wide range of spintronic devices and energy applications.

References

[1] Joe, M. et al. A comprehensive study of piezomagnetic response in $CrPS_4$ monolayer: mechanical, electronic properties and magnetic ordering under strains. J. Phys. Condens. Matter 29, (2017) 405801.

Figures

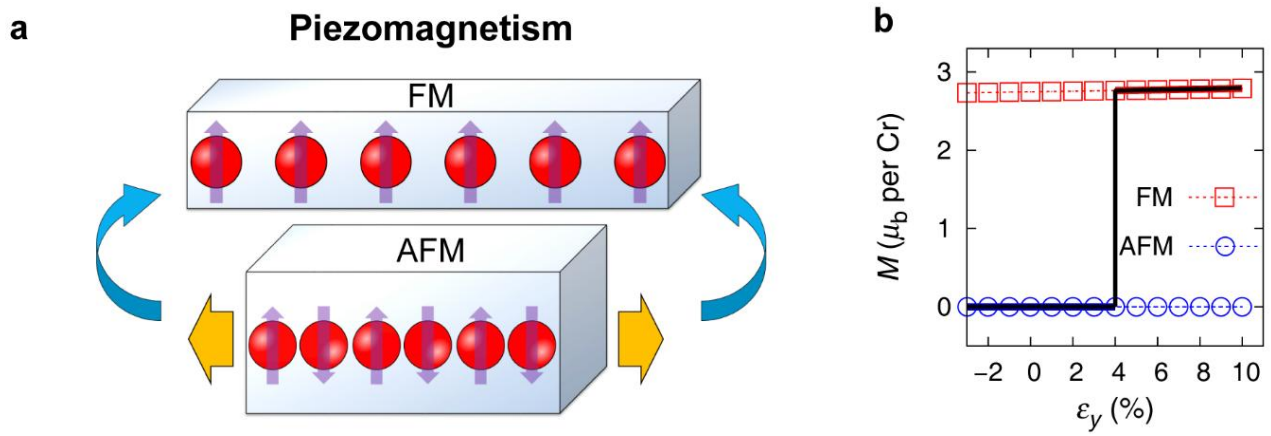

Figure 1: (a) A schematic diagram describing piezomagnetism. (b) Magnetization as a function of uniaxial strain ε_y.

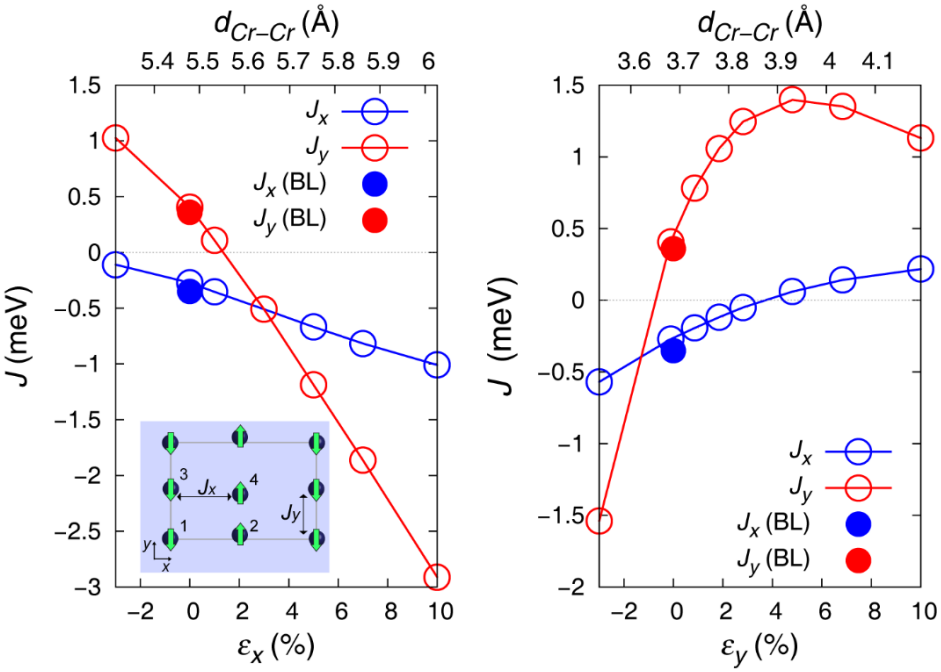

Figure 2: The exchange constants J of monolayer $CrPS_4$ as a function of applied uniaxial strain along the x (a) and y (b) directions. Filled circles at the zero-strain position indicate corresponding bulk values. (Inset) Collinear X-AFM order of Cr spins (arrows) in a unit cell (4 Cr atoms).