Catalogue of C-paired Spin-Valley Locking in antiferromagnetic materials

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C-paired spin-valley locking(SVL) refers that the spin and valley degree of freedoms are locked by the real space crystal symmetries. Materials with C-paired SVL can generate piezomagnetism(PZM) and large transverse spin current[1]. In this letter we propose the general theory of C-paired SVL and conclude 38 magnetic point groups that can host C-paired SVL considering spin-orbit coupling(SOC). Then we develop the algorithm to determine SVL structure in magnetic system. SVL is classified into collinear, coplanar, and spatial types and further generalized by elementary SVL group that protects SVL structure. At last, we proof that our algorithm can also classify other pseudovectors like berry curvature(Ω). Through first-principles calculations, the SVL and Ω distribution of CoF_2 and CrSb confirm our classification and further provide microscopic mechanisms to explain PZM and anomalous/valley Hall effect.

Following our algorithm and classification, 130 magnetic materials in MAGNDATA[2] are predicted to host C-paired SVL. Our work provides systematic classification of SVL in AFM materials with SOC and underpins the upcoming research of valleytronics, spintronics, and topological phase in AFM materials.

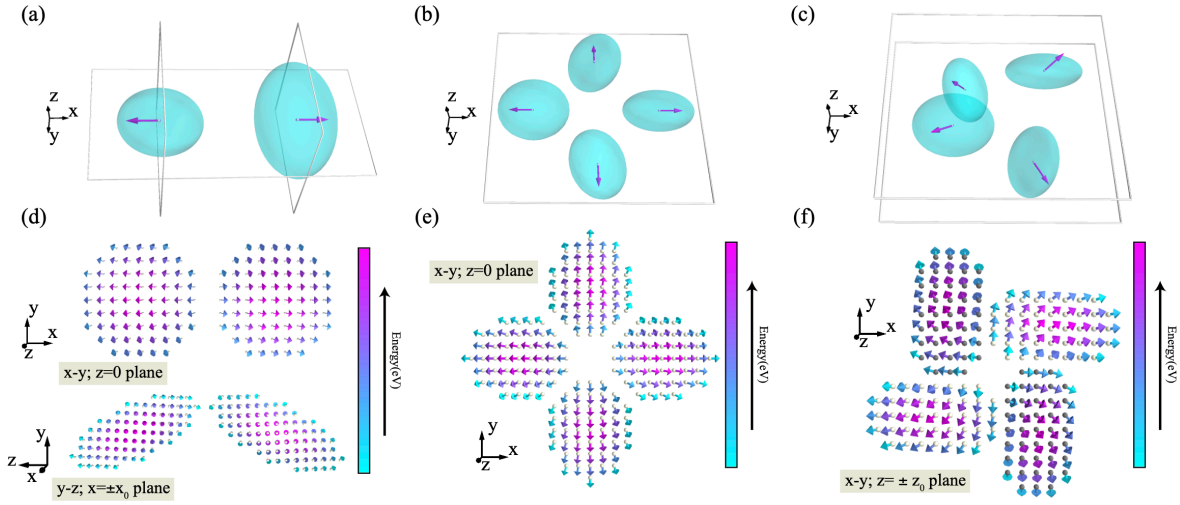

FIG. 1. Three types of SVL: (a,d) collinear SVL; (b,e) coplanar SVL; (c,f) spatial SVL. The light blue surfaces in each diagram represent the fermi surfaces and the location and orientation of purple arrows at the centre of each fermi surface represent the valley location and spin orientations.

[1] Ma H Y, Hu M, Li N, et al. Multifunctional antiferromagnetic materials with giant piezomagnetism and noncollinear spin current[J]. Nature communications, 2021, 12(1): 1-8.

[2] Gallego S V, Perez-Mato J M, Elcoro L, et al. MAGNDATA: towards a database of magnetic structures. I. The commensurate case[J]. Journal of Applied Crystallography, 2016, 49(5): 1750-1776.