First principle calculations of intrinsic Hall effect in $Sr_2FeMoO_{6-\delta}$ with oxygen nonstoichiometry

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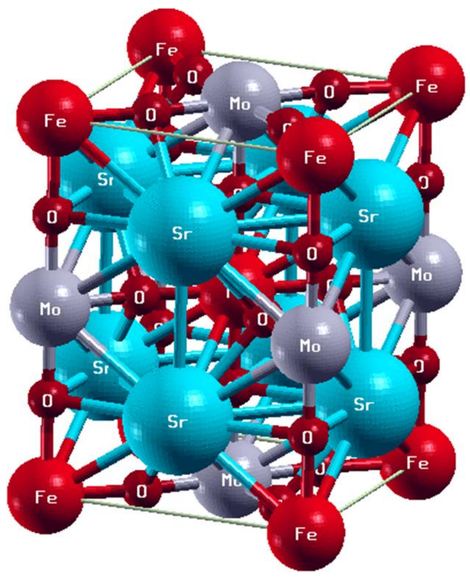
Introduction: To date new class of materials with nontrivial band structures such as Dirac and Weil topological semimetals attract scientific interest due to large anomalous Hall and Nernst effects in relatively low magnetic fields. The Sr_2FeMoO_6 is versatile double perobskite compound prospective for spintronic application, wherein magnetic and electronic properties can be easily tuned by degree of the antisite disorder of Fe and Mo cations, the oxygen nonstoichiometry or by introduction of secondary phase dielectric shells. This composite being ferrimagnet with high Curie temperature ~420 K has broken time-reversal symmetry and possibility of strong spin-orbital coupling (SOC), which are prerequisites for large intrinsic anomalous transport effects. Here investigation of $Sr_2FeMoO_{6-\delta}$ band structure, its topological features related to Berry curvature (BC) and intrinsic anomalous Hall conductivity (AHC) using first principle calculations are presented.

Methods: Basic self-consistent and non-self-consistent calculations of ground state density and Bloch wavefunctions in Sr_2FeMoO_6 required to determine DOS and ab-initio band structure were carried out using Quantum Espresso package. DFT calculations were performed using PBEsol pseudopotentials for Perdew-Burke-Ernzerhoff functional on Monkhorst-Pack *k*-points grid of 6x6x4. Maximally localized Wannier functions (MLWF) were extracted from band structure data using Wannier90 package. The Hamiltonian in the Wannier functions basis was employed for calculations of Berry curvature and AHC. Wannier procedure was used in two modes to find Berry curvature– with SOC and without it. The calculations were performed on Sr_2FeMoO_6 structure including 2 f.u.

Results:

Figure 1. I4/m crystalline structure of Sr_2FeMoO_6 below magnetic ordering T



Self-consistent + non-self-consistent DFT calculations

Magnetic moment per f.u. : Fe ~ 4.45 μ_B, Mo ~ -0.4 μ_B. 100% spin polarization, majority spin band gap of 0.5 eV. Mo 4d, Fe 3d, O 2p electron states prevail at the Fermi level of minority spin down bands

Figure 2. The density of states of Sr_2FeMoO_6.

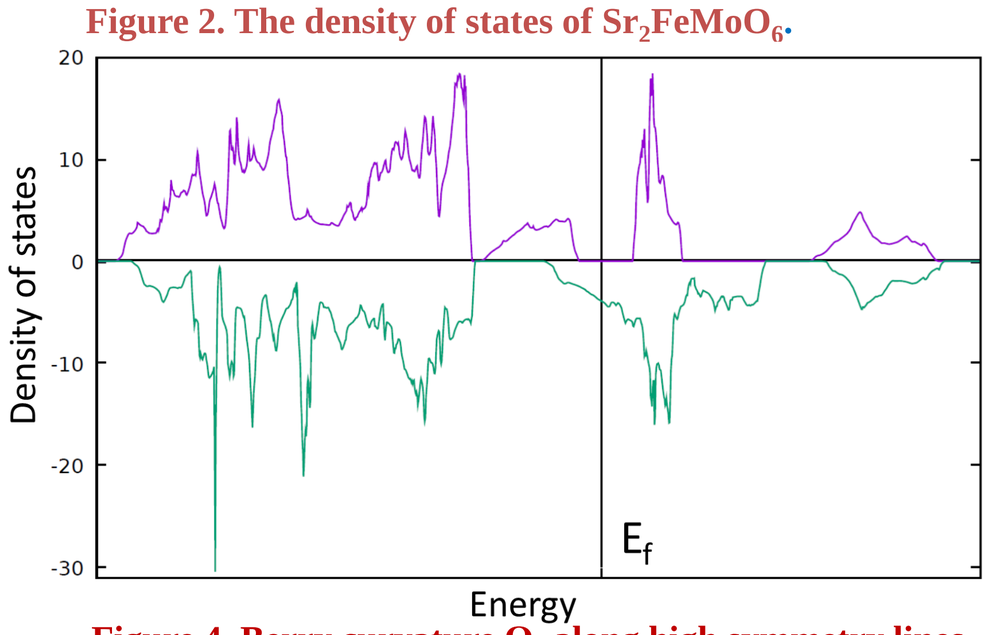
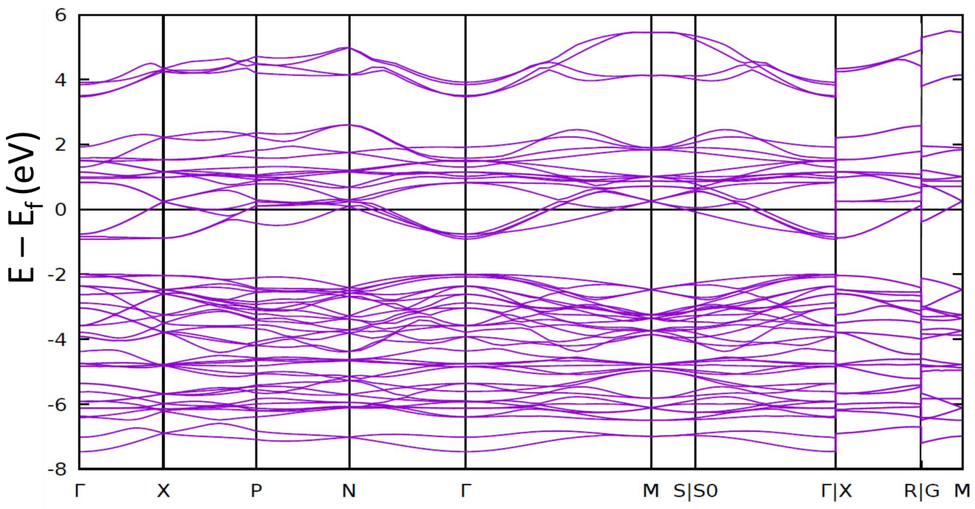


Figure 3. Spin down bands along high-symmetry points of Brillouin zone near the Fermi level

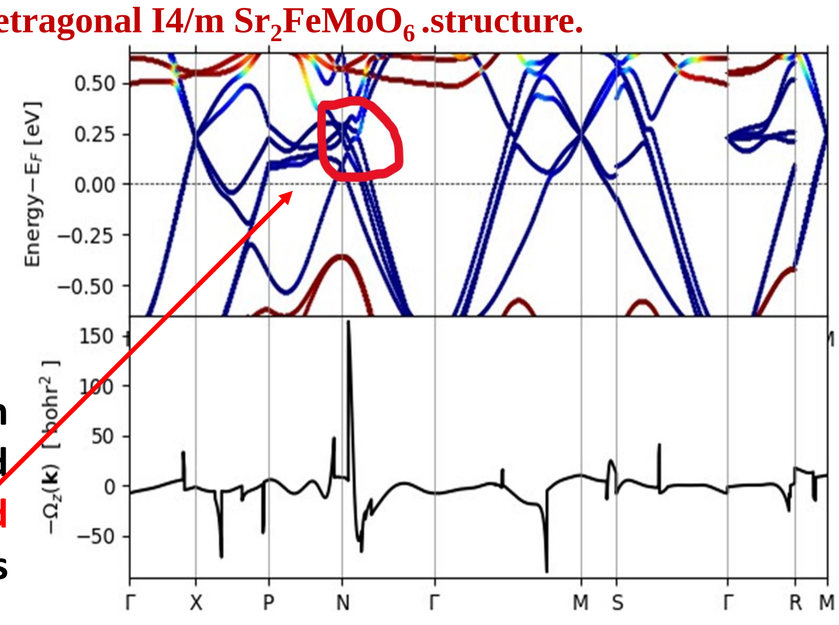


3 main mechanisms of AHC

- Side jump
- Skew scattering
- Berry curvature (intrinsic)

Berry curvature depends only on ideal crystal structure and concentrates around avoided crossings in k-space. SOC leads to enhancing Berry curvature

Figure 4. Berry curvature Ω_z along high symmetry lines of tetragonal I4/m Sr_2FeMoO_6 .structure.



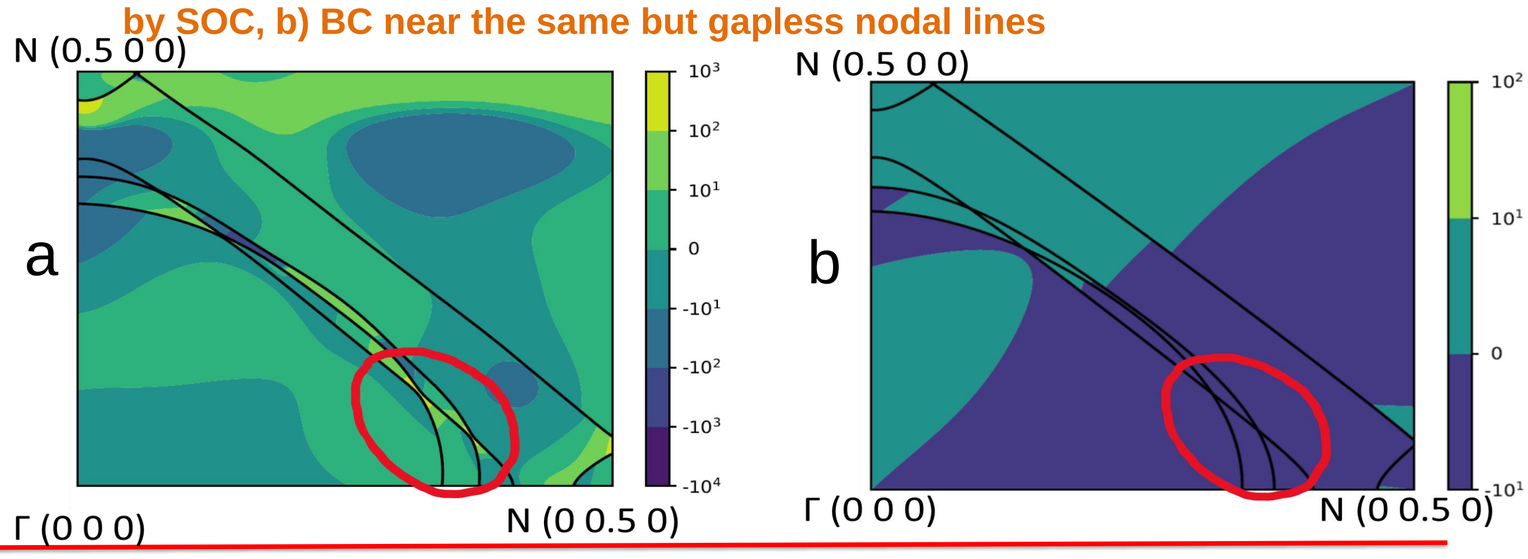
Wannier90 code AHC calculations based on integrating the Berry curvatures:

$$\sigma_{\alpha\beta} = -\frac{e^2}{\hbar}\int_{\mathrm{BZ}}\frac{d\boldsymbol{k}}{(2\pi)^3}\sum_n f_n(\boldsymbol{k})\Omega_{n,\alpha\beta}(\boldsymbol{k})$$

$$\Omega_{n,\alpha\beta}(\boldsymbol{k}) = -2\hbar^2\mathrm{Im}\sum_{m\neq n}\frac{v_{nm,\alpha}(\boldsymbol{k})v_{mn,\beta}(\boldsymbol{k})}{[\epsilon_m(\boldsymbol{k})-\epsilon_n(\boldsymbol{k})]^2}$$

n is the band index, α and β are the Cartesian coordinates x, y, z; α ≠ β for the AHC components, $f_n(k)$ is the occupation factors at the k point, n(k) is the eigenenergy for n-th band at a givenk point and $v_{nm}(k)$ is the matrix element of the velocity operator between the occupied n state and the unoccupied m state.

Figure 5. Berry curvature in the intersection of Fermi surface with the plane including Γ --- N lines: a)increase in BC near gapped nodal lines (Fig.4) split by SOC, b) BC near the same but gapless nodal lines



Conclusions:

- **The ground state of Sr_2FeMoO_6 possesses maximal spin polarization due to 0.5 eV band gap at the Fermi level in spin-up channel. Conductive spin-down states are mainly filled by Fe, Mo d and O 2p electrons. Total magnetization is about 4 μ_B/f.u., which is in accordance with theoretical value for stoichiometric composition.**
- **Band structure of Sr_2FeMoO_6 includes gapped nodal lines along Γ --- N direction in momentum space, which gap out with introduction of SOC. This topological band crossing allows to refer this compound to topological materials.**
- **Intrinsic AHC of the Sr_2FeMoO_6 due to BC reaches 44 S/cm, which is reasonably close to experimentally measured value of total AHC. It can be enhanced due to oxygen nonstoichiometry driven shift of Fermi energy upward by 0.25 eV to the level where gapped nodal lines are present.**