

FIG. 1. (Color online) The side views of schematic crystal structures of Fe_2I_2 (a) and Fe_2IBr (b).

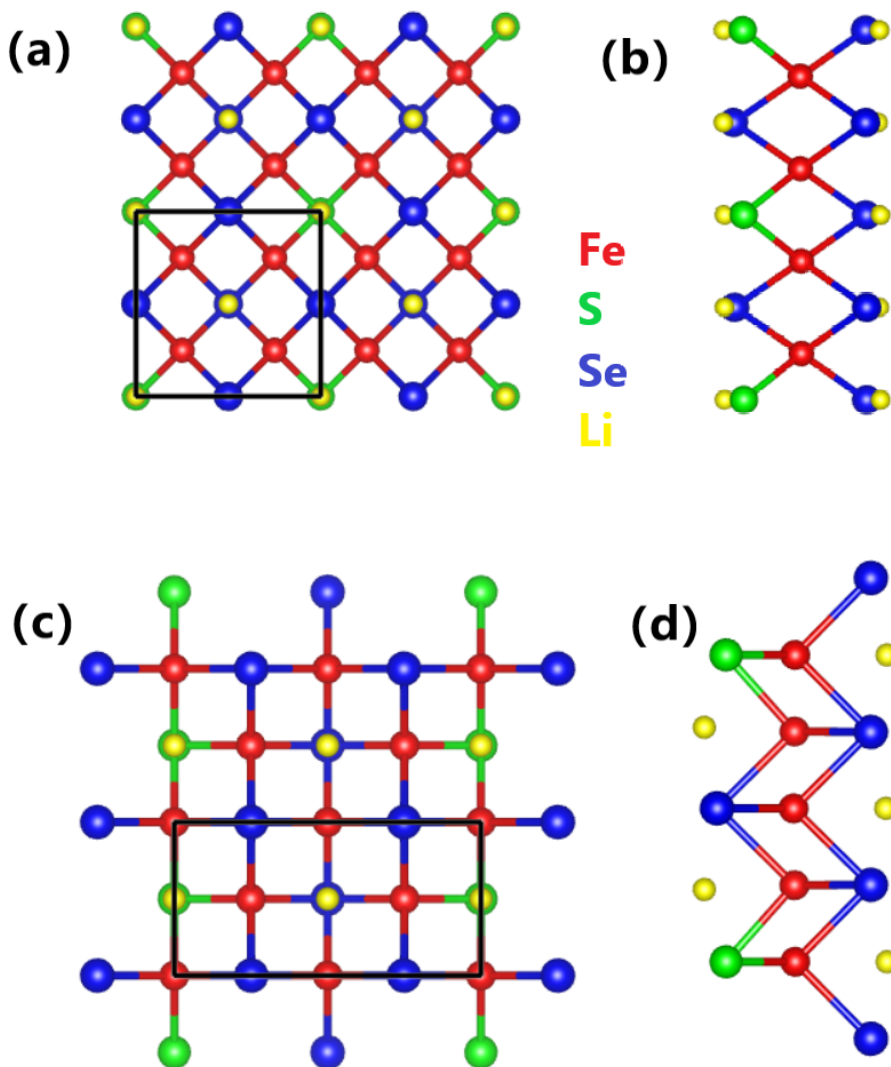


FIG. 2. (Color online) The top and side views of schematic crystal structures of $\text{LiFeSe}_{0.75}\text{S}_{0.25}$ with α (a,b) and β phases (c,d).

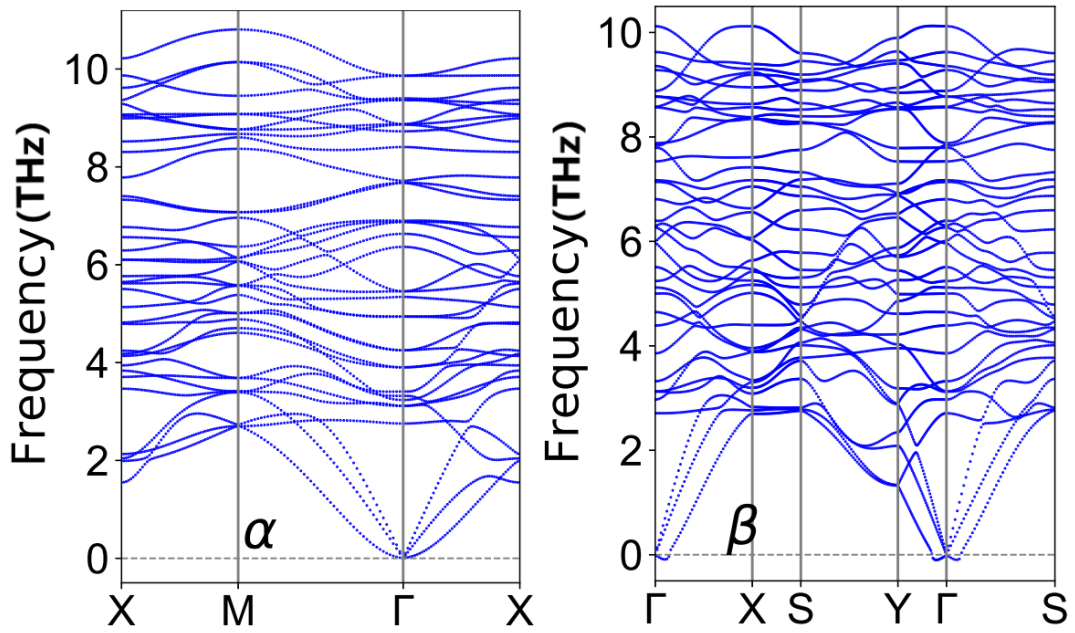


FIG. 3. (Color online) The phonon dispersions of monolayer $\text{LiFeSe}_{0.75}\text{S}_{0.25}$ with α and β phases.

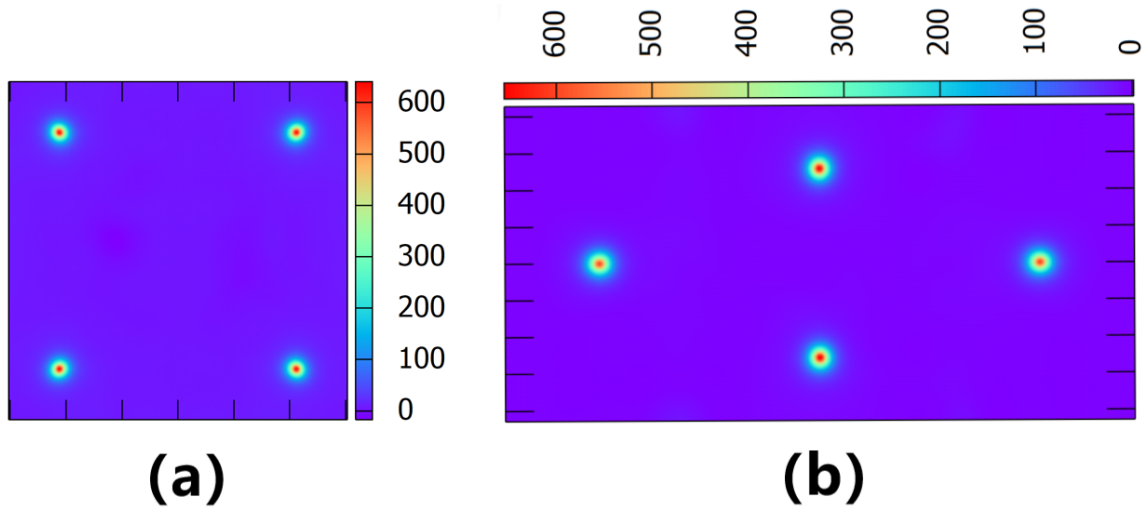


FIG. 4. (Color online) For monolayer $\text{LiFeSe}_{0.75}\text{S}_{0.25}$ with α (a) and β (b) phases, the distribution of Berry curvature contributed by occupied valence bands in the momentum space.

TABLE I. For monolayer $\text{LiFeSe}_{0.75}\text{S}_{0.25}$ with α and β phases, the lattice constants a_i in \AA , the elastic constants C_{ij} in Nm^{-1} , the piezoelectric strain coefficients d_{31} and d_{32} in pm/V , MAE in $\mu\text{eV}/\text{Fe}$, easy axis (EA), normalized exchange parameter J in meV and Curie temperature T_C in K .

Name	a_1	a_2	C_{11}	C_{22}	C_{12}	C_{66}	d_{31}	d_{32}	MAE	EA	J	T_C
α	5.19	5.19	100.80	100.80	17.88	29.04	-0.064	-0.064	176	c	129.54	950
β	7.33	3.67	88.76	89.41	30.11	41.11	-0.564	-0.011	191	c	131.81	966

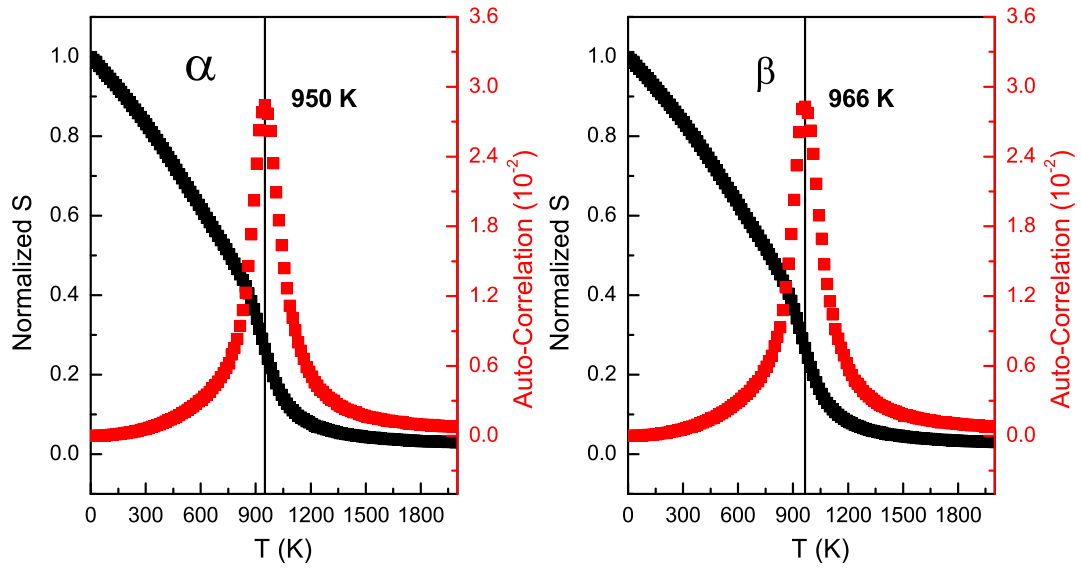


FIG. 5. (Color online) The normalized magnetic moment (S) and auto-correlation of monolayer $\text{LiFeSe}_{0.75}\text{S}_{0.25}$ with α and β phases as a function of temperature.