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Orbital frustration induced unusual ordering in semiconductor alloys[1] KAI LIU, Fudan Univ, WANJIAN YIN, Soochow Univ, SHIYOU CHEN, East China Normal Univ, XINGAO GONG, Fudan Univ, SUHUAI WEI, Computational Science Research Center, HONGJUN XIANG, Fudan Univ — It is well known that ternary zinc-blende semiconductors are always more stable in the chalcopyrite (CH) structure than the Cu-Au (CA) structure because CH structure has large Coulomb interaction and reduced strain energy. Surprisingly, an experimental study showed that $ZnFeSe_2$ alloy takes the CA order as the ground state structure, which is consistent with our density function theory (DFT) calculations showing that the CA order has lower energy than the CH order for $ZnFeSe_2$. We reveal that the orbital degree of freedom of high-spin Fe^{2+} ion (d^6) in the tetrahedral crystal field plays a key role in stabilizing the CA order. First, the spin-minority d electron of the Fe^{2+} ion tends to occupy the d_{x2-y2}–like orbital instead of the d_{3z2-r2}–like orbital because of its large negative Coulomb energy. Second, for a nearest-neighboring Fe^{2+} pair, two spin-minority d electrons with occupied d_{x2-y2}–like orbitals in the plane containing the Fe-Fe bond has lower electronic kinetic energy. Both conditions can be satisfied in the CA ordered $ZnFeSe_2$ alloy, while there is an orbital frustration in the CH structure. Our results suggest that orbital degree of freedom provides a new way to manipulate the structure and properties of alloys.

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