Abstract Submitted
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Magnetic interactions in FeSe studied by first principle calculations[1] SHUAI WANG, FA WANG, Peking Univ — Based on first principle calculations we have investigated the evolution of magnetism in free-standing monolayer FeSe with respect to lattice constant and magnetism in bulk FeSe. The computational results show that the magnetic order in free-standing monolayer FeSe will change from anti-ferromagnetic pair-checkboard order to stripe collinear order along with enlarging lattice constant. The magnetic order in bulk FeSe will change from stripe collinear order to anti-ferromagnetic pair-checkboard order only if structure reconstruction is allowed. We use J_1-J_2-K_1 model to fit the calculated total energies of different magnetic orders to study magnetic interaction strengths in FeSe. The fitting results of J_1-J_2-K_1 indicate that magnetic interactions in FeSe are quite strong and highly frustrated, and increase slowly with enlarging lattice parameter.

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