Effect of Interface on the Stability of Spin Density Wave in Monolayer FeSe Ultrathin Film Grown on SrTiO3

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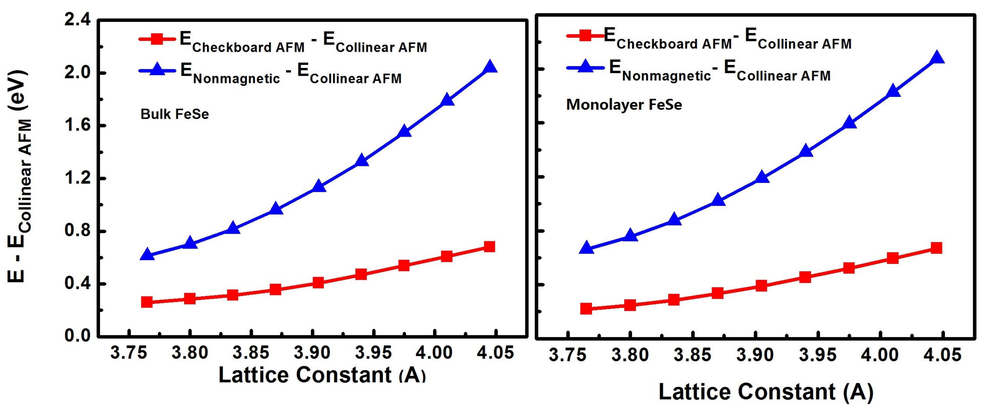
Abstract

Recently, monolayer FeSe grown on SrTiO3 substrate has been reported as one of the iron-based high temperature superconductors. The superconducting transition temperature **Tc** above 50 K and the sign of spin density wave (**SDW**) has been observed. In this work, by the first-principles calculations, we have theoretically studied how the interface affects the stability of SDW state in FeSe. We find with the expanding of the lattice constant due to the strain exerted by the substrate, the SDW state tends to be more stable in FeSe. The enhancement of antiferromagnetic superexchange interactions bridged by Se atoms causes the stabilization of the SDW state. Besides that, we find both the substrate SrTiO3 and the oxygen vacancies existing on the surface of SrTiO3 would suppress the stability of the SDW state. The oxygen-vacant substrate would dope charge to the monolayer FeSe and further destroy the SDW. All of our results are in good agreement with the experiments.

Calculation method

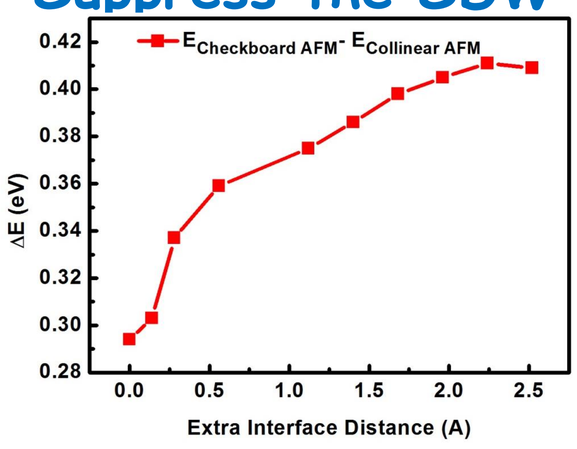
- **First principle calculation about electronic and magnetic properties: DFT+PAW-PBE with VASP code.**
- **The frustrated Heisenberg model from DFT calculation data is used to describe the magnetic property.**

Stability of SDW versus Strain



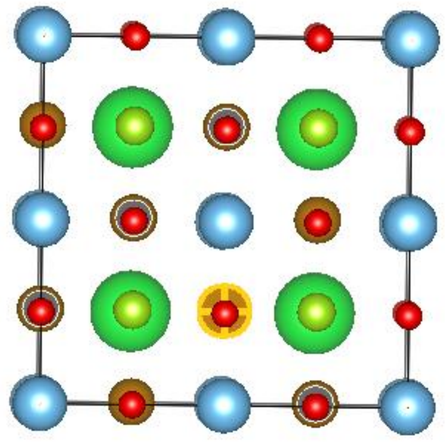
In both bulk and monolayer FeSe, SDW state tends to be stable with the expanding of the lattice . The enhance of the superexchange Fe-Se-Fe is the main reason.

Perfect SrTiO3 Interface Suppress the SDW

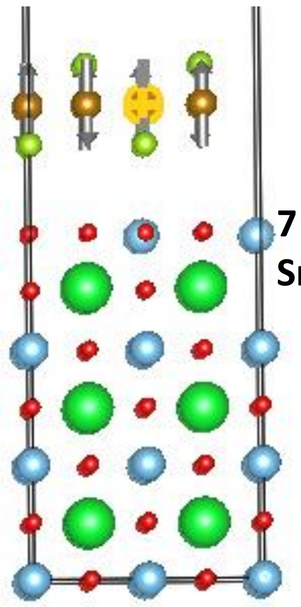


- **The perfect SrTiO3 almost shows no charge transfer to single Layer FeSe.**
- **The perfect interface would reduce the charge density on dxz/dyz orbital , it decreases the effect of superexchange and suppress the SDW.**

Simulation Structure



2 × 2 supercell



7 layers slab SrTiO3 substrate

Oxgyen-vacant Substrate Suppress the SDW

	$E_{Chk} - E_{Col}$ (eV)	Charge Doping in Chk FeSe	Charge Doping in Col FeSe
None O vac	0.294	0.000	0.000
12.5% O vac	0.173	0.489	0.376
25% O vac	0.153	0.715	0.518
50% O vac	0.143	0.827	0.644

With the increase of the number of oxygen vacancies, the energy difference between two AFM state would decrease while the charge doping to the monolayer FeSe would increase.

Conclusion

- **Strain would enhance the SDW in monolayer and bulk FeSe because the enhancement of the superexchange.**
- **The perfect interface would suppress the SDW by reduce the charge density on dxz/dyz orbital and decrease the superexchange effect.**
- **The oxygen vacancies would dope charge to FeSe and further suppress the SDW.**