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Electronic properties of Monolayer FeSe on CaF_2 via DFT

A recent study on FeSe thin films grown on different substrates revealed that films on CaF_2 substrate has the maximum T_c ˜15 K. However, the monolayer FeSe grown on $SrTiO_3$ (STO) substrate generated much research interest when superconductivity was observed at T_c above 100 K by means of *in situ* four-point probe electrical transport measurements. There are different factors that were identified, such as the tensile strain and electron doping, which contributed to the enhancement of the T_c. To investigate the interface effect in the superconductivity of monolayer FeSe, we calculated the structural and electronic properties of monolayer FeSe grown on CaF_2. Only electron pockets are observed around the M point for both NM and AFM configurations. The same feature is observed in experimental studies on 1ML FeSe/STO. This suggests that the mechanism of superconductivity of single-layer FeSe on STO and CaF_2 might be the same. However, further experimental research on 1ML FeSe/CaF_2 is necessary to verify our results.

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