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Interplay of magnetic order and defect modulation in mononlayer FeSe[1] JUNQIANG LU, University of Puerto Rico at Mayaguez, PENGFEI ZHANG, JIAN WU, Tsinghua University — We investigate the role of the defects (vacancy and anti-site) at the Fe-site on the magnetic order in monolayer FeSe. Experimental STM studies of defect states reveal that two type dumbbell-like dimers are formed at the surface of monolayer FeSe. We perform first-principles calculations of the magnetic structure of FeSe monolayer in the presence of defects in order to identify the origin of the STM observations. We consider various distribution of the defects and compare the checkerboard and collinear antiferromagnetic orders. Our results show that a single defect can give a dimer in STM image. A preliminary analysis show that both dimers are centered at the defects with their bright ends positioned on two adjacent Se atoms. We show that the two magnetic orders give rise to two distinct dimers types, in agreement with experiments.

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