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Chalcogen-height dependent magnetic interactions in iron chalcogenide superconductors CHANG-YOUN MOON, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Korea — We have investigated the magnetic properties of iron chalcogenide superconductors using the first-principles pseudopotential method. It is found that the stability of magnetic phases is very sensitive to the height of chalcogen atoms from the Fe plane: while FeTe with optimized Te height exhibits the double stripe magnetic ordering, the single stripe ordering becomes the ground state phase when Te height is lowered below a critical value by, e.g., Se doping. This behavior is understood by opposite Te-height dependences of the strength of superexchange interactions among nearest and next nearest neighbor iron atoms, and a longer-range magnetic interaction mediated by itinerant electrons. We also demonstrate a linear temperature dependence of the macroscopic magnetic susceptibility in the single stripe phase in contrast to a constant behavior in the double stripe phase. Compared with known experimental observations, our results suggest a comprehensive and unified view in the magnetism and the superconductivity in iron-based superconducting materials. This work was supported by NRF of Korea (Grant No. 2009- 0081204) and KISTI Supercomputing Center (Project No. KSC-2008-S02-0004).

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