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Role of Hydrogen in the Electronic Properties of H-rich Pnictide Superconductors YINA HUANG, University of California Davis, XIANGLONG YU, DAYONG LIU, Institute of Solid State Physics, Chinese Academy of Sciences, LIANGJIAN ZOU, University of Science and Technology of China — The electronic and magnetic properties of the parent material CaFeAsH and its La/Co-doped compounds are investigated using first-principles calculations based on the generalized gradient approximation (GGA). We predict that the ground state of CaFeAsH is a spin-density-wave (SDW)-type striped antiferromagnet driven by Fermi surface nesting. We find a sandglass-type hole pocket near the Γpoint in CaFeAsH that is not present in CaFeAsF. In comparison with CaFeAsF, the sandglass-shaped pocket, mainly contributed from Fe d_{xz}+d_{yz} orbitals, arises from the weak oxidization of CaH layers and the hybridization enhancement between FeAs layers. In contrast, the electronic properties of electron doped $Ca_{0.75}La_{0.25}FeAsH$ and $CaFe_{0.75}Co_{0.25}AsH$ indicate that La or Co doping almost does not affect the sandglass-type Fermi surface, while the suppression of Fermi surface nesting in $Ca_{0.75}La_{0.25}FeAsH$ is weaker than that in $CaFe_{0.75}Co_{0.25}AsH$. This features may contribute to the higher T_c in La-substituted CaFeAsH.

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