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Doping-induced suppression and reemergence of magnetism in $\text{LaFeAsO}_{1-x}\text{H}_x$: A DFT+DMFT study CHANG-YOUN MOON, Korea Research Inst of Standards and Science (KRISS) — Recently, hydrogen doped 1111 material, $\text{LaFeAsO}_{1-x}\text{H}_x$ is shown to exhibit another superconducting phase followed by a new antiferromagnetic phase at high doping levels. In this study, we investigate the magnetic and electronic properties of these materials using DFT+DMFT method, which captures the material-specific electronic correlation. Considering changes of both electron occupancy and lattice structure caused by the hydrogen doping which turn out to have the opposite effects on the electron correlation and magnetism, we find that both the magnetic moment and local susceptibility initially decrease to the minimum at around $x = 0.3$ and then increase again up to $x = 0.6$, in agreement with the experimental phase diagram of two separate AFM phases centered at $x = 0$ and 0.5 . More electron occupation at $d_{xz/yz}$ orbitals with the doping enhances the importance of the d_{xy} orbital in the static magnetic moment and also in spin dynamics, while reducing the orbital polarization. Our results emphasize the importance of the electron correlation and structural modification in understanding the doping induced evolution of the electronic structure, and also the magnetism as an indispensable ingredient for the emergence of the superconductivity in these materials.

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