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A Study of Hydrogen Anion Substitution in 1111-type Iron Arsenides

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Hydrogen is the simplest bipolar element and its valence state can be controlled from +1 to −1. We have synthesized the 1111-type iron arsenides CaFeAsH and LnFeAsO1−xHx (Ln = lanthanide; $0 \leq x \leq 0.5$) with the ZrCuSiAs type structure by a high-pressure synthesis method. The position and valence state of the substituted H were determined by neutron diffraction and density functional theory calculations. The close similarity in the structural and electrical properties of CaFeAsH and CaFeAsF indicated the formation of the hydride ion (H−), which is isovalent with the fluoride ion (F−), in the 1111-type iron arsenides. When some of the O2− ions in LnFeAsO are replaced by H−, superconductivity is induced by electron doping to the FeAs-layer to maintain charge neutrality. Since the substitution limit of hydrogen in LnFeAsO ($x \approx 0.5$) is much higher than that of fluorine ($x \approx 0.2$), the hydrogen substitution technique provides an effective pathway for high-density electron-doping, making it possible to draw the complete electronic phase diagram of LnFeAsO. The x-T diagrams of $\mathrm{LnFeAsO}_{1-x}\mathrm{H}_x$ (Ln = La, Ce, Sm, Gd) have a wide superconducting (SC) region spanning the range x = 0.04 to 0.4, which is far from the parent antiferromagnetic region near x = 0.0. For $\mathrm{LaFeAsO}_{1-x}\mathrm{H}_x$, another SC dome region was found in the range x = ∼ 0.2 to ∼ 0.5 with a maximum Tc = 36 K, in addition to a conventional SC dome located at x ∼ 0.08 with maximum Tc = 29 K. Density functional theory calculations performed for $\mathrm{LaFeAsO}_{1-x}\mathrm{H}_x$ using virtual crystal approximation indicated that the newly observed Tc is correlated with the appearance of degeneration of the Fe 3d bands (dxy, dyz and dzx), which is caused not only by regularization of the tetrahedral shape of FeAs_4 due to chemical pressure effects but also by selective band occupation with doped electrons. Very recently, a new AFM phase was found around x=0.5, suggesting that the double dome Tc structure reflects the presence of two AFM phases at x=0 and 0,5. In this talk, I review the recent progress in superconductivity in 1111-type iron (oxy)arsenides and related compounds induced by hydrogen anion substitution.