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First-principles study of light-element doping effects on iron-based superconductors HIROKI NAKAMURA, MASAHIKO MACHIDA, Japan Atomic Energy Agency — Since the discovery of the iron-based superconductor, $\text{LaFeAsO}_{1-x}\text{F}_x$ whose T_c reached 26K, various types of iron-based superconductors have been fabricated to attain higher T_c . Recently, it is reported that T_c of an iron-based superconductor LaFeAsO_{1-y} is enhanced to 35K by doping hydrogen. This result implies that atoms of light elements penetrate into the crystal of iron-based superconductors and transform their structures into more useful ones for superconductivity. In this talk, we investigate how the light elements are doped in the iron-based superconductors by using the first-principles density functional theory. Furthermore, we evaluate the effects of doping on the crystal structures and electronic states and explore the origin of the T_c enhancements.

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