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General Rule of Negative Effective Ueff System & Materials Design of High-Tc Superconductors by ab initio Calculations HIROSHI KATAYAMA-YOSHIDA, AKITAKA NAKANISHI, HIROKI UEDE, YUKI TAKAWASHI, TETSUYA FUKUSHIMA, KAZUNORI SATO, Osaka University — Based upon ab initio electronic structure calculation, I will discuss the general rule of negative effective U system by (1) exchange-correlation-induced negative effective U caused by the stability of the exchange-correlation energy in Hund's rule with high-spin ground states of d5 configuration, and (2) charge-excitation-induced negative effective U caused by the stability of chemical bond in the closed-shell of s2, p6, and d10 configurations. I will show the calculated results of negative effective U systems such as hole-doped CuAlO2 and CuFeS2. Based on the total energy calculations of antiferromagnetic and ferromagnetic states, I will discuss the magnetic phase diagram and superconductivity upon hole doping. I also discuss the computational materials design method of high-Tc superconductors by ab initio calculation to go beyond LDA and multi-scale simulations.

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