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**How to design negative effective $U$ Fermion system in hole doped chalcopyrite CuFeS$_2$?** HIROSHI KATAYAMA-YOSHIDA, TETSUYA FUKUSHIMA, HIROKI UEDE, YUKI TAKAWASHI, AKITAKA NAKANISHI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University — Here, we have proposed a general rule of the attractive Fermion system in the purely electronic origin, which is called negative effective $U$ ($U_{eff} < 0$) system. Purely electronic-originated $U_{eff} < 0$ is caused by (i) the exchange-correlation-induced energy gain in the Hund's rules, and (ii) the charge-excitation-induced energy gain. Based on the general design rules, we perform ab initio electronic structure calculations for hole-doped Chalcopyrite CuFeS$_2$. It is found that the hole-doped CuFeS$_2$ has the negative $U_{eff} = -0.44$ eV (-5000 K). The $U_{eff} < 0$ in CuFeS$_2$ is originated by the charge-excitation- induced mechanism in the hole-doped Cu$^{2+}$($d^9$) and S$^{2-}$($s^2p^5$), and also originated by the exchange-correlation-induced mechanism in the hole-doped Fe$^{4+}$($d^4$). The hole-doped paramagnetic and metallic CuFeS$_2$ with the $U_{eff} < 0$ may cause a possible super-high-$T_c$ superconductor ($T_c \approx 1000$ K, if $2\Delta/k_BT_c = 10$ by assuming a strong coupling regime.) because of the strong attractive electron-electron interactions (superconducting gap $\Delta \approx |U_{eff}| \approx 5000$ K). We propose a new computational materials design methodology to design super-high-$T_c$ superconductors starting from the atomic number only.

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