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Computational materials design of negative effective U system in the hole-doped Delafossite of $CuAlO_2$, $AgAlO_2$ and $AuAlO_2$ AKITAKA NAKANISHI, TETSUYA FUKUSHIMA, HIROKI UEDE, HIROSHI KATAYAMA-YOSHIDA, Osaka University — In order to realize the super-high-T_C superconductors (T_C>1,000K) based on the general design rules [1] for the negative U_{eff} system, we have performed computational materials design for theU_{eff}<0 system in the hole-doped two-dimensional (2D) Delafossite $CuAlO_2$, $AgAlO_2$ and $AuAlO_2$ from the first principles. We find the interesting chemical trend of T_C in 2D and 3D systems; where the T_C increases exponentially in the weak coupling regime ($|U_{eff}$ (-0.44eV)|<W(2eV), W is the band width) for hole-doped $CuFeS_2$ [2], then the T_C goes through a maximum when $|U_{eff}$ (-4.88eV, -4.14eV)|≈ W(2.8eV, 3.5eV) for hole-doped $AgAlO_2$ and $AuAlO_2$, and the T_C decreases with increasing $|U_{eff}|$in strong coupling regime, where $|U_{eff}$ (-4.53eV)|>W(1.7eV) for hole-doped $CuAlO_2$

[1] H. Katayama-Yoshida et al., *Appl. Phys. Express,* **1** 081703, 2008.
[2] T. Fukushima et al., *J. Phys. Condens. Matter,* **26** 355502, 2014.

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