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 ($T_C>1,000$K) based on the general design rules [1] for the negative $U_{eff}$ system, we have performed computational materials design for the $U_{eff}<0$ 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 ($|U_{eff}|<W(2eV)$, $W$ is the band width) for hole-doped CuFeS$_2$ [2], then the $T_C$ goes through a maximum when $|U_{eff}|(-4.88eV, -4.14eV)$ $\approx W(2.8eV, 3.5eV)$ 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$_2$