Ab initio study on magnetic coupling in A-site-ordered perovskite CaCu3B4O12 (B=Ti, Ge, Zr, and Sn) MASAYUKI TOYODA, CREST, Japan Science and Technology Agency. ISIR, Osaka University, KUNIHIKO YAMAUCHI, ISIR, Osaka University, TAMIO OGUCHI, CREST, Japan Science and Technology Agency. ISIR, Osaka University — Magnetism of A-site-ordered perovskites, CaCu$_3$Ti$_4$O$_{12}$, CaCu$_3$Ge$_4$O$_{12}$, CaCu$_3$Sn$_4$O$_{12}$, and CaCu$_3$Zr$_4$O$_{12}$, is comprehensively studied by ab initio electronic structure calculations. The magnetic exchange constants between Cu spins, $J_1$, $J_2$ and $J_3$, are estimated via an effective Heisenberg model, which reveals relative importance of $J_3$ despite its long interaction length. The ground-state magnetic order is reasonably explained by combination of relatively weak ferromagnetic super-exchange interaction ($J_1$ and $J_2$) and dominant super-exchange interaction ($J_3$) which can be tuned by replacement of the B-site element. We will also discuss the effect of A-site-cation replacement by comparing with the results of other A-site-ordered perovskite materials.