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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, $CaCu_3Ti_4O_{12}$, $CaCu_3Ge_4O_{12}$, $CaCu_3Sn_4O_{12}$, and $CaCu_3Zr_4O_{12}$, 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.

Masayuki Toyoda
CREST, Japan Science and Technology Agency,
Gobancho, Chiyoda-ku, Tokyo, 102-0076 Japan

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