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Theoretical study of SrRu2O6 and related compounds[1] SATOSHI OKAMOTO, Oak Ridge National Lab, MASAYUKI OCHI, Department of Physics, Osaka University, RYOTARO ARITA, RIKEN Cen- ter for Emergent Matter Science (CEMS), JIAQIANG YAN, Oak Ridge National Lab, NANDINI TRIVEDI, Department of Physics, The Ohio State University — We theoretically investigate the electronic property of a hexagonal compound $SrRu_2O_6$ and isostructural $CaOs_2O_6$ [1]. Here, we focus on the topological property of these compounds under various strain conditions. Based on an analysis of parity eigenvalues, we anticipate that a three-dimensional strong topological insulating state should be realized when band inversion is induced at the A point in the hexagonal Brillouin zone. We found that such a transition is indeed possible in these compounds under certain strain conditions. In particular, for $CaOs_2O_6$, the transition could be induced more easily than $SrRu_2O_6$ owing to the stronger spin-orbit coupling and smaller lattice constants. We also investigate the magnetic property of $SrRu_2O_6$ using density functional theory. Detailed comparison with experimental reports [2,3] will be presented. [1] M. Ochi *et al.*, Phys. Rev. B **93**, 195149 (2016). [2] W. Tian *et al.*, Phys. Rev. B **92**, 100404(R) (2015). [3] C. I. Hiley *et al.*, Phys. Rev. B **92**, 104413 (2015).

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