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First-principles calculation of Ca2RuO4 at high pressure NOBUMI MIYAWAKI, TATSUYA SHISHIDOU, Hiroshima University, TAMIO OGUCHI, Osaka University — It has been observed that the layered perovskite antiferromagnetic insulator Ca_2RuO_4 reveals a phase transition into a ferromagnetic metal at 0.5GPa [1]. This insulator-metal transition is accompanied by a structural change with tilt and rotation of RuO_6 octahedron within the space group *Pbca*. Above about 9GPa, another transition from the ferromagnetic to superconducting phase has been recently reported [2]. The transition includes a structure change from *Pbca* to *Bbcm*. In this study, a first-principles calculation is performed to study the electronic structure of Ca_2RuO_4, especially focusing on the changes of Ru 4*d* states, with pressure. As the pressure is increased, calculated ferromagnetic spin moment of Ru is gradually decreased in *Pbca* owing to the widening of Ru 4*d* band. It is interesting that a ferromagnetic solution still exists in *Bbcm*. Similar structural changes (the tilt and rotation of RuO_6 octahedron) take place in $Ca_{2-x}Sr_xRuO_4$, where orbital hybridization with spin-orbit coupling (SOC) is crucial [3]. We also investigated effects of SOC, with the result that those appear even in the electronic structure of Ca_2RuO_4. Calculation results optimizing the structure will be also discussed. [1] F. Nakamura, et al., Phys. Rev. B **65**, 220402(R) (2002). [2] P. L. Alireza, *et al.*: J. Phys.: Condens. Matter **22**, 052202 (2010). [3] T. Oguchi, J. Phys. Soc. Jpn. **78**, 044702 (2009).

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