First-principles calculation of Ca$_2$RuO$_4$ at high pressure

NOBUMI MIYAWAKI, TATSUYA SHISHIDOU, Hiroshima University, TAMIO OGUCHI, Osaka University — It has been observed that the layered perovskite antiferromagnetic insulator Ca$_2$RuO$_4$ 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$_2$RuO$_4$, especially focusing on the changes of Ru $4d$ 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 $4d$ 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$_x$RuO$_4$, 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$_2$RuO$_4$. 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).