Rashba splitting and spin-valley coupling in ferroelectric oxides

Kunihiko Yamauchi¹, Paolo Barone², Silvia Picozzi²

¹) ISIR-Sanken, Osaka University, Japan
²) CNR-SPIN, Italy

Corresponding author: Kunihiko Yamauchi (kunihiko@sanken.osaka-u.ac.jp)

Spin-orbit coupling is responsible for the Rashba effect and spin-valley coupling in the absence of structural inversion symmetry. Although such effects are usually found at surfaces, it was recently suggested they might also occur in polar (ferroelectric) bulk materials. For example, GeTe shows a strong bulk Rashba effect in its polar rhombohedral structure. In our first-principles study, we propose novel bulk Rashba effects and spin-valley coupling in newly designed perovskite oxide heterostructures. Aiming at a sizable spin splitting, low-spin 5d transition metal ions are embedded in host ferroelectric oxides with LiNbO₃-type polar distortion. Our calculations clarify that the spin-orbit coupling largely splits 5d orbital states of the transition metal ion into |j> states, which are further split into different spin states, due to breaking of inversion symmetry. In this talk, the microscopic mechanism for the Rashba effect and the spin-valley coupling in our novel oxide systems will be discussed. If time permits, Rashba-like spin-splitting phenomena in antiferromagnetic ferroelectric oxides will also be introduced.

This work is supported by a Grant-in-Aid for Young Scientists (B) from the Japan Society for the Promotion of Science (No 26800186).