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First Principles Study on Topological-Phase Transition in Ferroelectric Oxides KUNIHIKO YAMAUCHI, ISIR-Sanken, Osaka University, Japan, PAOLO BARONE, Graphene Labs, Istituto Italiano di Tecnologia, Italy, SILVIA PICOZZI, Consiglio Nazionale delle Ricerche (CNR-SPIN), Italy — Graphene is known as a 2D topological insulator with zero energy gap and Dirac cone. In this study, we theoretically designed a honeycomb structure of Au ions embedded in a ferroelectric host oxide, in order to exploit structural distortions to control topological properties. We show that the polar structural distortion induces the emergence of spin-valley coupling, together with a topological transition from a quantum spin-Hall insulating phase to a trivial band insulator. The phase transition also affects the Berry curvature and spin-valley selection rules. Analogously to graphene, the microscopic origin of this topological phase is ascribed to a spin-valley-sublattice coupling, which arises from the interplay between trigonal crystal field and an "effective" spin-orbit interaction due to virtual excitations between e_g and t_{2g} states of transition-metal ions.

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