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Possible Strong Topological Insulator Phase in Li_2IrO_3 HEUNG SIK KIM, CHOONG HYUN KIM, Department of Physics and Astronomy and Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747, Korea, HOSUB JIN, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA, JAEJUN YU, Department of Physics and Astronomy and Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747, Korea — Recently Na_2IrO_3, a layered $5d$ transition metal oxide compound, was suggested to be a possible topological insulator (TI) based on the $j_{eff} = 1/2$ states induced by the strong spin-orbit coupling of Ir $5d$ states, but its realization has not been clarified yet. In search of the TI phase in transition metal oxides, we propose Li_2IrO_3 to be a candidate for the three-dimensional strong TI. By carrying out Wannier function analysis based on first-principles calculations, we constructed a low energy effective Hamiltonian, which leads to a three-dimensional extension of the Kane-Mele model with third-nearest-neighbor hopping within the Ir honeycomb layer and a significant inter-layer coupling. The nature of spin-orbit coupled states near the Fermi level depends on the change of the trigonal crystal field driven by the lattice deformations. A competition between the third next-nearest-neighbor hopping parameter and the trigonal crystal field is found to play a key role in determining the topological character of Li_2IrO_3.

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