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Theoretical study of phase transition from normal to topological insulators in Na_2IrO_3 CHOONG HYUN KIM, HEUNGSIK KIM, HOGYUN JEONG, Seoul National U., Seoul, Korea, HOSUB JIN, Northwestern U., Evanston, IL, USA, JAEJUN YU, Seoul National U., Seoul, Korea — Recently Na_2IrO_3 has been suggested to have possible quantum spin Hall effect arising from the novel $j_{\rm eff} = 1/2$ state of $5d$ Ir atoms. The electronic structure of the layered iridium oxides with honeycomb lattice is investigated based on a tight-binding model with spin-orbit coupling included. Our tight-binding model, fitted to the first-principles calculation results, reveals that the electronic states near the Fermi level are not the $j_{\rm eff} = 1/2$ states but the e'_g states. The delocalized $5d$ orbitals lying in the edge sharing octahedron structure leads to (i) a significant direct hopping between neighboring Ir $5d$ states, (ii) a strong trigonal crystal field, and (iii) non-negligible next-nearest-neighbor and next-next-nearest-neighbor hoppings. A peculiar band structure is found to play a crucial role in determination of the topological nature of the spin-orbit coupled ground state in Na_2IrO_3.

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