Theoretical study of phase transition from normal to topological insulators in $\text{Na}_2\text{IrO}_3$

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 $\text{Na}_2\text{IrO}_3$ has been suggested to have possible quantum spin Hall effect arising from the novel $j_{\text{eff}} = 1/2$ 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 $j_{\text{eff}} = 1/2$ 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 5$d$ 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 $\text{Na}_2\text{IrO}_3$. 

Choong Hyun Kim
Seoul National U., Seoul, Korea

Date submitted: 17 Dec 2009