Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Molecular orbital polarization in $Na_2Ti_2Sb_2O$: a scenario to metal-to-metal phase transition without spontaneous symmetry breaking

HEUNG-SIK KIM, HAE-YOUNG KEE, Univ of Toronto — We suggest a scenario of partial Fermi surface (FS) gapping related to metal-to-metal phase transition without a spontaneous symmetry breaking. This theory is applied to $Na_2Ti_2Sb_2O$, where the density polarization of spin-orbital entangled molecular orbitals occurs due to spin-orbit coupling. This is further enhanced by electronic correlations of Ti d-orbitals. Sharp increase of the polarization happens above a critical electronic interaction strength which then gaps out a part of FS made of d-orbitals, while the rest of FS associated with Sb p-orbitals remain almost intact. Experimental implications to test our proposal are also discussed.

Heung Sik Kim
Univ of Toronto

Date submitted: 03 Nov 2015 Electronic form version 1.4