Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Ab-initio study on crystal structure of $\alpha$-$RuCl_3$** HAE-YOUNG KEE, HEUNG-SIK KIM, Univ of Toronto — $\alpha$-$RuCl_3$ was recently proposed as a candidate system for materialization of Kitaev model, but precise structural information of the compound has remained elusive. For the clarification of the full three-dimensional crystal structure of $\alpha$-$RuCl_3$, we performed ab-initio electronic structure calculations including effects of spin-orbit coupling (SOC) and electron correlations. We found that SOC prevents dimerization between Ru atoms, and keeps the system close to honeycomb lattice. The ground state crystal structure has monoclinic $C2/m$-type layer stacking, but trigonal $P3_112$-and orthorhombic $Cmc2_1$-type stacking orders are comparable to the $C2/m$ structure in energy, so that stacking faults can be easily introduced. The electronic structure and the $j_{\rm eff}$=1/2 pseudospin exchange interactions and possible magnetic states in $\alpha$-$RuCl_3$ will be presented.

Heung Sik Kim
Univ of Toronto

Date submitted: 03 Nov 2015 Electronic form version 1.4