



Contribution ID: 62

Type: **Talk**

## **【608】 Non-trivial band topology in high pressure structure of $\text{Ba}_3\text{CaIr}_2\text{O}_9$**

*Thursday 30 August 2018 16:00 (15 minutes)*

Iridium oxides with  $d^5$  configuration have attracted considerable interest in the last decade due to the realisation of spin-orbit-coupled (SOC)  $j_{eff} = 1/2$  insulating ground states. Recently, a new class of  $5d^4$  iridates with a singlet ( $j_{eff} = 0$ ) ground states have been realised in  $(\text{Ba}/\text{Sr})_2\text{YIrO}_6$ . Here, we propose a new honeycomb lattice compound  $\text{Ba}_3\text{CaIr}_2\text{O}_9$  in the  $j_{eff} = 0$  class of materials. Using ab initio methods including many-body wavefunction calculations we characterise the SOC ground and excited states and show that a  $j_{eff} = 0$  singlet ground state is realised. Further, we find that the material hosts non-trivial electronic band structure with a well defined  $Z_2$  topological invariant. We analyse the effect of electronic correlations on the non-trivial bands using the Gutzwiller wavefunction approach.

**Primary author:** KATUKURI, Vamshi Mohan (EPFL)

**Co-authors:** Dr WU, Quansheng (EPFL); YAZYEV, Oleg (EPFL - EPF Lausanne)

**Presenter:** KATUKURI, Vamshi Mohan (EPFL)

**Session Classification:** Advances in Topological Materials

**Track Classification:** Advances in Topological Materials