

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Singular manifestation of square-planar coordination of an iridate Na_4IrO_4 ¹ SUDIPTA KANUNGO, BINGHAI YAN, PATRICK MERZ, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARTIN JANSEN, Max-Planck-Institut für Solid State Research, Stuttgart, Germany — Local environments and valence electron counts primarily determine the electronic states and physical properties of transition metal complexes. For example, square-planar surroundings found in transition oxometalates such as Curprates, Nickaltes are usually associated with the d^8 or d^9 electron configuration. In this work, we address an experimentally observed exotic square-planar mono-oxoanion $[\text{IrO}_4]^{4-}$ in Na_4IrO_4 with Ir(IV) in d^5 ($S=\frac{3}{2}$ state) configuration, using ab-initio calculations. On contrary, in its 3d counterpart, Na_4CoO_4 , Co(IV) is in tetrahedral coordination with $S=\frac{5}{2}$ high spin state. Our ab-initio calculations reveal that the on-site Coulomb interaction U is the essential factor for determining the stability of the local coordination as well as spin state. We find that due to weak Coulomb repulsion of Ir-5d electrons, Na_4IrO_4 form in a square-planar coordination whereas for Na_4CoO_4 , Co(IV) is in tetrahedral coordination, due to strong electron correlation at 3d Co site. Following the trend from 5d to 3d, we predict that the intermediate 4d material Na_4RhO_4 , if synthesized, may favor tetrahedral coordination but with an $S=\frac{1}{2}$ low spin state.

¹Sudipta Kanungo, Binghai Yan, Patrick Merz, Claudia Felser and Martin Jansen. *Angew. Chem. Int. Ed.* 54, 5417 (2015).

Sudipta Kanungo
Max Planck Institute for Chemical Physics of Solids

Date submitted: 04 Nov 2015

Electronic form version 1.4