On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

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KO_2: Realization of Orbital Ordering in a p-Shell System

Most of the experimental efforts probing magnetism, charge and orbital ordering have concentrated on transition metal compounds. Possible examples among p band systems have not been explored. The first step in this direction would be to search for narrow band materials in which Coulomb interactions should be important. If one could engineer magnetism in these materials, one could generate a new class of compounds with a rich phase diagram as their transition metal counterparts. Our search for stoichiometric materials with p shell magnetism led us to an unusual set of oxides formed by the alkali metal atoms (A) [1]. Here we have considered the prototypical example of KO_2 and explore its properties in greater detail [2].

KO_2 is a molecular solid consisting of oxygen dimers aligned parallel in a body centred tetragonal lattice at high temperatures. K present in the lattice donates an electron which goes on to occupy the O p levels. As the basic electronic structure is similar to that of an oxygen molecule, except for broadening due to solid state effects, KO_2 represents the realization of the doping of oxygen molecules arranged in a lattice. These considerations alone result in magnetism with high ordering temperatures as our calculations reveal. However, we find that the high temperature structure is unstable to an orbital ordering (OO) transition. The microscopic considerations driving the OO transition, however, are electrostatic interactions instead of the often encountered super-exchange driven ordering within the Kugel-Khomskii model [3] often used to describe the OO. This OO transition is also found to preclude any possibility of high magnetic ordering temperatures, which otherwise seemed possible.

[1] W. Hesse, M. Jansen and W. Schnick Prog. Solid. St. Chem. 19 (1989) 47.
[2] Ashis Kumar Nandy, Priya Mahadevan, P. Sen and D.D. Sarma. Phys. Rev. Lett. 105 (2010) 056403 .
[3] K. I. Kugel and D. I. Khomskii Sov. Phys. JETP 37 (1973) 725.

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