MS17-05 **Discovery of novel post-perovskites by high pressure methods.** Martin Bremholm,[ab] S. E. Dutton,[bc] P. W. Stephens[d], R. J. Cava,[b] [a]*Dept. of Chemistry, Aarhus University, Denmark,* [b]*Dept. of Chemistry, Princeton University, USA,* [c]*Cambridge University, England,* [d] *Department of Physics, SUNY, Stony Brook NY, USA*
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We have prepared a novel post-perovskite, $NaIrO_3$, by high pressure solid state synthesis and recovered it to ambient conditions [1]. Among the few known oxide post-perovskites, $NaIrO_3$ is the first example with a pentavalent cation. The structure consists of layers of corner- and edge-sharing IrO_6 octahedra separated by layers of NaO_8 bicapped trigonal prisms. $NaIrO_3$ shows no magnetic ordering and resistivity measurements show non-metallic behaviour. The crystal structure, electrical and magnetic properties are discussed and compared to known post-perovskites and pentavalent perovskite metal oxides.

In 2004 two groups independently discovered a high pressure transition at 125 GPa in $MgSiO_3$ from a perovskite to a post-perovskite structure [2,3]. The transition is believed to explain the observed transition in the speed of sound in the Earth's lower mantle and it is of high importance in seismology. Considering the extreme pressure required to study $MgSiO_3$ there is a great interest in discovering analog compounds which are stable at lower pressures. The recent discoveries of several new oxide post-perovskites have also sparked interest in the materials science community regarding their electronic and magnetic properties. The interest is further invigorated by the valence flexibility of the cations allowing mixed valence and tuning of properties.

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MS18-01 **Electron properties of pharmaceutical molecules.** Nour Eddine Ghermani,[a,b] Nouha El Hassan,[a,b] Jean-Michel Gillet,[b] Nicolas Guiblin,[b] Anne Spasojevic-de Biré,[b] [a]*Laboratoire de Physique Pharmaceutique UMR CNRS 8612, Université Paris Sud 11, Faculté de Pharmacie, 5, rue Jean-Baptiste Clément, 92296 Châtenay-Malabry, France,* [b]*Laboratoire Structures, Propriétés et Modélisation des Solides (SPMS) UMR CNRS 8580, Ecole Centrale Paris, 1, Grande Voie des Vignes, 92295 Châtenay-Malabry, France.*
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Beyond the conventional crystal structures, electron and electrostatic properties can be derived experimentally from high resolution X-ray diffraction data. For more than thirty years, this experimental approach has been successfully applied to different kinds of compounds. Results are comparable to those obtained from high standard quantum mechanics methods. When a molecule crystallizes in different forms (polymorphism), it gives the opportunity to study the subtle re-arrangement of the electron distribution in relation with the crystal environment and the intermolecular interactions. In the presentation, we will focuse on a small and flexible pharmaceutical molecule, piracetam (2-oxo-1-pyrrolidineacetamide) which is the first nootropic agent discovered. The characterization of physical and chemical properties of polymorphs is of considerable importance particularly for the pharmaceutical research and development. It deals with therapeutic treatments based on the solid drug formulations which largely dominate all other galenic preparations. Polymorphism has a great impact not only on the industrial processing (powder formulations, tablets) but also on the drug bioavailability in relation with solubility, permeability etc. The crystallographic studies are pertinent in this field of research since they reveal the arrangement of the molecules in the crystal lattice. The electrostatic interactions, from which the macroscopic properties (both thermodynamically stable and metastable states) originate, are related to the molecular arrangements, packing, hydrogen bonding and contacts.[1] Several properties as electron density, atomic charges, electrostatic potential and forces will be presented and discussed.

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