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# PEROVSKITES FULL OF SURPRISES

Mardi 19 décembre 2017 à 10h30  
Salle 2

### Biography

Artem Abakumov graduated from the Department of Chemistry at Moscow State University in 1993 and obtained his PhD in Chemistry from the same University in 1997. He spent about three years as a postdoctoral fellow and invited professor in the Electron Microscopy for Materials Research (EMAT) laboratory at University of Antwerp and joined EMAT as a research leader in 2008. Since 2015 he holds a Full Professor position at Skolkovo Institute of Science and Technology (Skoltech) in Moscow. His research is focused at crystal and defect structures of inorganic solids and linking this knowledge to designing new materials and getting deeper insight into their functional properties. His interests comprise materials for metal-ion batteries, magnetic and ferroelectric complex oxides, incommensurately modulated and composite structures, conventional and multidimensional crystallography, structure analysis using a combination of transmission electron microscopy, synchrotron X-ray and neutron powder diffraction.

### Abstract

Perovskite-based oxides have inspired a series of amazing discoveries in material science, and still remain a playground for solid state chemistry and condensed matter physics. Extensive research during last few decades revealed rich crystallography and crystal chemistry of perovskite-based structures with distortions of different origins – cooperative octahedral tilting distortion, charge/orbital ordering, (anti) polar displacements, cation/anion ordering – and their combinations. However, highly unusual and amazingly complex perovskite structures can still be found beyond the commonly accepted picture. Relaxing the rigid unit mode for the  $BX_6$  octahedra may lead to broken corner-sharing connectivity of the octahedral framework and non-cooperative tilting distortion modes, realized in some double perovskites and elpasolites [1]. Competing off-center displacements due to second-order Jahn-Teller effect and octahedral rotations/tilts lead to incommensurately modulated structures with frustrated octahedral tilting distortion in layered A-site ordered perovskites, such as  $Li_{3x}Nd_{2/3-x}TiO_3$  and many others [2, 3]. Coupling of octahedral tilting distortion, octahedral deformation and strongly covalent Bi-O bonding results in antiferrodistortive modulated structures in isovalent A- and B-site substituted  $BiFeO_3$  [4, 5]. Finally, anion deficiency in the perovskites with lone-pair A-cations can be realized through the crystallographic shear plane mechanism, previously unforeseen for perovskites with occupied A-positions, as demonstrated by heterovalent substitutions in  $BiFeO_3$  and  $PbTiO_3$  and new perovskite-based  $AnBnO_{3n-2}$  homologous series [6 - 8].

### References

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- [6] A. Abakumov et al., *Chem. Mater.*, 23, 255 (2011).
- [7] D. Batuk et al., *Angew. Chem.*, 54, 14787 (2015).
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