

**MS26-O2** Incommensurate oxides and sulfidesBerthold Stöger<sup>1</sup>

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The defining property of a crystal has for a long time been its three-dimensional periodicity. With the advent of X-ray diffraction, a seemingly equivalent property of crystals emerged, namely their discrete diffraction pattern. But already in 1927 Dehlinger [1] observed sharp "lattice ghosts" in cold-formed metals, which are incompatible with lattice periodicity. These additional reflections emerge from structural modulations of a basic structure with an incommensurate periodicity.

The superspace approach [2] provides the necessary theoretical foundation to conveniently describe such incommensurately modulated phases and their diffraction patterns. It resulted in an explosion of the number of known incommensurates [3] and the realization that quasiperiodicity is distinctly less rare than one might expect. Nevertheless, the existence of incommensurates still appears mysterious and counterintuitive.

To demonstrate the ubiquity and variety of these phases, several incommensurate oxides and sulfides are presented. The thortveitite family is made up of transition metal diphosphates, diarsenates or divanadates with the general formula  $M_2X_2O_7$  ( $X=P, As, V$ ). The members feature a complex crystal chemistry with commensurately and incommensurately modulated phases. The modulation is a dynamic phenomenon as evidenced by a complex phase transition behavior. Analogous phenomena are observed in the condensed phosphates and arsenates  $Tl_3P_3O_{14}H_8$  and  $Rb_3AlAs_3O_{12}$  and the orthophosphate  $K_3PO_4 \cdot 3H_2O$ .

In the ditellurates(IV)  $MTe_2O_8$  ( $M=Ca, Sr, Cd$ ) and their solid solutions, on the other hand, modulation is due to an occupational modulation of the O atoms. Accordingly, these phases do not feature structural phase transitions. Such complex static occupational modulations are likewise observed in natural sartorite and roschinite sulfosalts. Here, the modulation periodicities depend on subtle variations of the composition.

[1] U. Dehlinger, *Am. Mineral.* **1927**, 65, 615.[2] P. M. De Wolff, *Acta Crystallogr.* **1974**, A30, 777.[3] H. Z. Cummin, *Phys. Rep.* **1990**, 185, 211.

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**MS26-O3** Structural phase transitions in the organic-inorganic hybrid perovskitesSébastien Pillet<sup>1</sup>, Bendeif El Eulmi<sup>1</sup>, Yangui Aymen<sup>2,3</sup>, Triki Smail<sup>1</sup>, Abid Younes<sup>3</sup>, Boukheddaden Kamel<sup>2</sup>

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Organic-inorganic hybrid perovskites have recently emerged as highly efficient optoelectronic materials, and are being intensively investigated and developed for high performance photovoltaics, photodetections, light-emitting diodes and laser devices. These materials exhibit a structural topology derived from the  $ABX_3$  perovskite structure, consisting of a corner-sharing  $BX_6$  octahedral network completed by organic A cations. Depending on the size of the organic cation, 3D, 2D, and 1D systems have been reported.

The compounds  $(C_6H_{11}NH_3)_2[PbX_4]$  ( $X=I, Br, Cl$ ) exhibit a 2D structural architecture with semi-conducting inorganic layers of corner-sharing  $PbX_6$  octahedra separated by bilayers of  $C_6H_{11}NH_3^+$  cations. The optical properties (absorption and photoluminescence) have been investigated as a function of temperature, and show very interesting and unusual behaviors, such as white light emission, which are connected to structural phase transitions [1-3]. Single crystals of the three compounds and of the solid solutions  $(C_6H_{11}NH_3)_2[PbI_xBr_{4-x}]$  have been investigated through x-ray diffraction as a function of temperature. The corresponding structural phase diagram is very rich, displaying a different sequence of commensurate-incommensurate phase transitions for the bromine and iodine derivatives, characterized by a distortion and modulation of the inorganic perovskite layer. The mixed-halide series  $(C_6H_{11}NH_3)_2[PbI_xBr_{4-x}]$  obtained by gradual substitution of Br by I exhibits a morphotropic structural transition, which allows tuning the optical properties.

The complete structural phase diagrams and phase transitions will be described and discussed in connection to the temperature dependence of optical properties.

## References

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