

### MS15-P32 A high-temperature molecular ferroelectric Zn/Dy complex exhibiting single-ion magnet behavior and lanthanide luminescence

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Multifunctional molecular ferroelectrics are exciting materials synthesized using molecular chemistry concepts, which may combine a spontaneous electrical polarization, switched upon applying an electric field, with another physical property. Herein we report an example of a high temperature ferroelectric material based on a chiral Zn<sup>2+</sup>/Dy<sup>3+</sup> complex exhibiting Dy<sup>3+</sup> luminescence, optical activity and magnetism. We investigate the correlations between the electric polarization and the crystal structure and between the low temperature magnetic slow relaxation and the optical properties [1].

[1] J. Long, J. Rouquette, J.-M. Thibaud, R.A.S. Ferreira, L.D. Carlos, B. Donnadiou, V. Vieru, L.F. Chibotaru, L. Konczewicz, J. Haines, Y. Guari, J. Larionova, A high-temperature molecular ferroelectric zn/dy complex exhibiting single-ion-magnet behavior and lanthanide luminescence, *Angewandte Chemie (International ed. in English)*, 54 (2015) 2236-2240.

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### MS15-P33 Structural characterisation of stoichiometric and off-stoichiometric Cu<sub>2</sub>ZnSn(S<sub>x</sub>Se<sub>1-x</sub>)<sub>4</sub> by neutron diffraction

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Quaternary Cu<sub>2</sub>ZnSn(S<sub>1-x</sub>Se<sub>x</sub>)<sub>4</sub> compounds are promising semiconductor materials for absorber layer in thin film solar cells due to direct band gap in the range 1-1.5 eV and high absorption coefficient (>10<sup>4</sup>cm<sup>-1</sup>) [1,2]. All constituents of these films are abundant, low cost and non-toxic. The highest conversion efficiency of Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> solar cell is till now 12.6% [3]. In spite of previously reported stannite type structure for CZTSe, CZTS and CZTSe crystallize both in the kesterite type structure (space group ) [4,5]. A differentiation between the isoelectronic cations Cu<sup>+</sup> and Zn<sup>2+</sup> and consequently kesterite and stannite type structures is not possible using X-ray diffraction due to their similar scattering factors. But neutrons diffraction can solve this problem; the coherent scattering lengths are sufficiently different for these cations. It was shown by this method that both Cu<sub>2</sub>ZnSnS<sub>4</sub> and Cu<sub>2</sub>ZnSnSe<sub>4</sub> occur in the kesterite structure [6]. A detailed structural analysis of stoichiometric as well as off-stoichiometric Cu<sub>2</sub>ZnSn(S<sub>1-x</sub>Se<sub>x</sub>)<sub>4</sub> powder samples grown by solid state reaction, was performed by neutron diffraction. Rietveld refinement of neutron diffraction data using the FullProf suite software [7] lead to accurate values of lattice constants and site occupancy factors. From the latter the average neutron scattering length was derived which has given insights into the cation distribution within the crystal structure of stoichiometric as well as off-stoichiometric samples from Cu<sub>2</sub>ZnSn(S<sub>1-x</sub>Se<sub>x</sub>)<sub>4</sub> solid solution with different x values. The correlated information about changes in lattice parameters and cation site occupancies, details on the existing intrinsic point defects and their amounts obtained by neutron diffraction will be discussed. Acknowledgments: Financial supports from IRSES PVICOKEST 269167 and KESTCELLS 316488, FP7-PEOPLE-2012 ITN, Multi-ITN is highly appreciated. [1] J.M. Raulot, et al., *J. Phys. Chem. Solids* **66** (2005) 2019. [2] P.A. Fernandes et al., *Phys. Status Solidi C* **7** (2010) 901. [3] Wang, et al., *Adv. Energy Mater.* (2014), **4**, 1301465. [4] S.Schorr, *Solar Energy Materials and Solar Cells*, **95** (2011)1482. [5] S. Schorr, H.-J. Hoebler, and M. Tovar, *Eur. J. Mineral.* **19**, 1 (2007). [6] Siebentritt, S. and Schorr, S. *Prog. Photovolt: Res. Appl.*, **20**, 512 (2012) [7] Juan Rodriguez-Carvajal and Thierry Roisnel, [www.ill.eu/sites/fullprof/](http://www.ill.eu/sites/fullprof/)

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