

## Poster Presentation

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### *Fluorides containing lanthanides and yttrium at extreme conditions*

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We are interested in crystal structures and stabilities of fluoride materials containing lanthanides and yttrium that are related to the CaF<sub>2</sub> structure. These compounds are laser hosts and luminescent materials, oxygen sensors as well as components of solar cells. They exhibit various schemes of (dis)ordering of cations and anions in fluorite superstructures and anion-excess fluorites. In the last few years, we have performed a series of studies on the bulk AMF<sub>4</sub> and MF<sub>3</sub> materials (A = Li, Na, K; M = Y, lanthanide) at different pressure-temperature conditions. Among them, ordered LiYF<sub>4</sub> is a commercial host for solid state lasers, while partially ordered NaYF<sub>4</sub> doped with lanthanides is the most efficient material for green and blue up-conversion known to date. In the system KF–YF<sub>3</sub>, we have studied not only KYF<sub>4</sub> [1] but also KY<sub>3</sub>F<sub>10</sub>, which is an anion-excess 2×2×2 superstructure of fluorite at atmospheric conditions. At high temperatures and high pressures, it converts to another fluorite superstructure with disordered fluorine atoms. The pressure-induced LaF<sub>3</sub> post-tysonite structure is another example of the anion-excess fluorite [2]. Our work on the fluorite-related materials at extreme conditions provides information on their structural instabilities that could further be used to better understand and control their materials properties. For instance, we demonstrated that the NaMF<sub>4</sub> up-converters are unstable and that the ordering of the cations and vacancies in their structure is a slow process [3]. Consequently, the order–disorder transformations have a profound influence over the luminescent properties of these materials when doped.

[1] A. Grzechnik, K. Friese, *Dalton Trans.* 2013, 42, 441-447., [2] W.A. Crichton, P. Bouvier, B. Winkler, A. Grzechnik, *Dalton Trans.* 2010, 39, 4302-4311., [3] A. Grzechnik, K. Friese, *Dalton Trans.* 2012, 41, 10258-10266.

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