Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supporting Information:

Lanthanide luminescence as a local probe in mixed anionic hydrides – A case study on Eu^{2+}-doped $RbMgH_xF_{3-x}$ and $KMgH_xF_{3-x}$

Thomas Wylezich,[a] Sacha Welinski, [b] Markus Hölzel,[c] Philippe Goldner[b] and Nathalie Kunkel *[a]

[a] Chair for Inorganic Chemistry with Focus on Novel Materials, Department of Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85747 Garching, Germany. *E-mail: nathalie.kunkel@lrz.tu-muenchen.de
[b] Chimie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris, 11 rue Pierre et Marie Curie, 75005 Paris, France.
[c] Heinz Maier-Leibnitz-Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany.

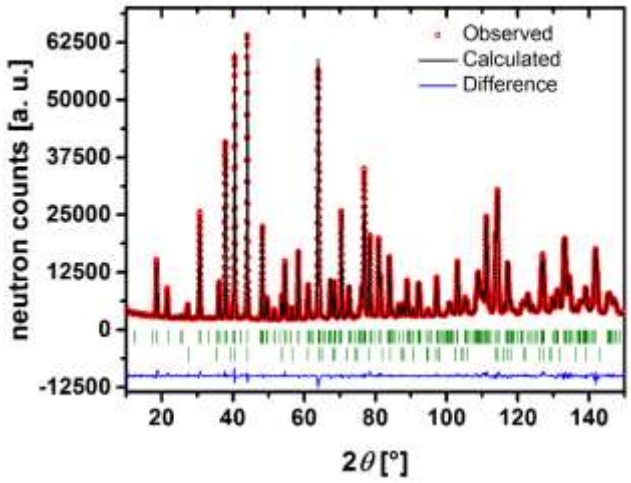

Figure S1. Rietveld refinement of the crystal structure of $RbMgD_{0.5}F_{2.5}$ from neutron diffraction data recorded at RT. Bragg markers from top to bottom $RbMgD_{0.5}F_{2.5}$ (95.1(3) wt-%) and MgF_2 (4.9(1) wt-%).

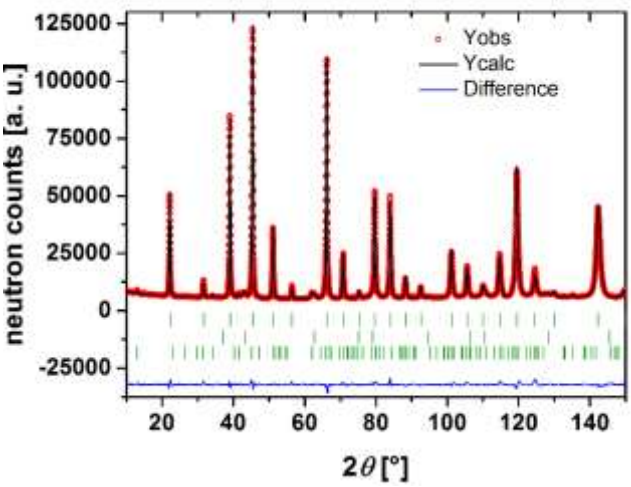

Figure S2. Rietveld refinement of the crystal structure of $KMgD_2F$ from neutron diffraction data recorded at RT. Bragg markers from top to bottom $KMgD_2F$ (83.6(2) wt-%), MgO (13.9(1) wt-%) and $K_2MgF_{4-x}H_x$ (2.5(1) wt-%).

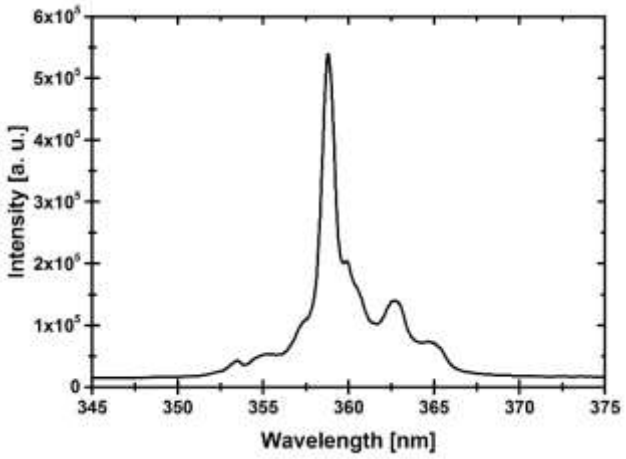

Figure S3. Higher resolution luminescence emission spectrum of $RbMgF_3:Eu^{2+}$ (0.5 at-%) at RT, excitation at 254 nm.

Table S1. Refined lattice parameters and atomic parameters for $RbMgD_{3-x}F_x$. Lattice parameters from high-resolution neutron data; atomic parameters and occupancy parameters from simultaneous refinement of X-ray and neutron data.

$RbMgD_3$		a = 5.9097(4) Å, c = 14.3315(11) Å, V = 433.5(5) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
Rb1	4*f*	1/3	2/3	0.0964(6)	0.872(17)	1
Rb2	2*b*	0	0	1/4	0.679(26)	1
Mg1	4*f*	1/3	2/3	0.6536(7)	0.441(16)	1
Mg2	2*a*	0	0	0	0.646(30)	1
D1	12*k*	0.1662(16)	2x	0.5800(4)	1.561(9)	1
D2	6*h*	0.5238(16)	2x	1/4	1.471(16)	1
$RbMgD_2F$		*a* = 5.8879(5) Å, *c* = 14.3067(13) Å, *V* = 429.5(5) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
Rb1	4*f*	1/3	2/3	0.0964(5)	0.918(17)	1
Rb2	2*b*	0	0	1/4	0.984(24)	1
Mg1	4*f*	1/3	2/3	0.6534(7)	0.662(17)	1
Mg2	2*a*	0	0	0	0.649(26)	1
D1/F1	12*k*	0.1655(15)	2x	0.5799(3)	1.395(12)	0.60(12) D / 0.40(12)F
D2/F2	6*h*	0.5234(14)	2x	1/4	1.354(18)	0.72(16) D / 0.28(16) F
$RbMgDF_2$		*a* = 5.8582(4) Å, *c* = 14.2571(10) Å, *V* = 423.7(5) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
Rb1	4*f*	1/3	2/3	0.0974(5)	0.638(14)	1
Rb2	2*b*	0	0	1/4	0.709(23)	1
Mg1	4*f*	1/3	2/3	0.6532(7)	0.390(15)	1
Mg2	2*a*	0	0	0	0.399(24)	1
D1/F1	12*k*	0.1660(13)	2x	0.5797(3)	0.877(10)	0.20(14) D / 0.80(17) F
D2/F2	6*h*	0.5218(14)	2x	1/4	0.855(17)	0.45(3) D / 0.55(3) F
$RbMgD_{0.5}F_{2.5}$		*a* = 5.8492(4) Å, *c* = 14.2397(12) Å, *V* = 421.9(5) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
Rb1	4*f*	1/3	2/3	0.0979(4)	0.505(14)	1
Rb2	2*b*	0	0	1/4	0.625(2)	1
Mg1	4*f*	1/3	2/3	0.6528(6)	0.287(14)	1
Mg2	2*a*	0	0	0	0.233(2)	1
D1/F1	12*k*	0.1663(13)	2x	0.5797(3)	0.746(8)	0.10(10) D / 0.90(10) F
D2/F2	6*h*	0.5212(13)	2x	1/4	0.575(15)	0.10(14) D / 0.90(14) F
$RbMgF_3$		*a* = 5.8421(3) Å, *c* = 14.2206(9) Å, *V* = 420.3(4) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
Rb1	4*f*	1/3	2/3	0.0987(5)	0.597(16)	1
Rb2	2*b*	0	0	1/4	0.700(26)	1
Mg1	4*f*	1/3	2/3	0.6526(7)	0.381(17)	1
Mg2	2*a*	0	0	0	0.309(27)	1
F1	12*k*	0.1663(14)	2x	0.5796(4)	0.737(9)	1
F2	6*h*	0.5207(16)	2x	1/4	0.602(14)	1

Table S2: Refined lattice parameters for $RbMgF_{3-x}D(H)_x$ are used in Fig. 3.

x	$RbMgF_{3-x}D_x$ (neutron data)			$RbMgF_{3-x}H_x$ (X-ray data)		
	a [Å]	c [Å]	V [Å^3]	a [Å]	c [Å]	V [Å^3]
0	5.8421(3)	14.2206(9)	420.3(4)	5.8375(2)	14.2108(9)	419.4(2)
0.5	5.8492(4)	14.2397(12)	421.9(5)	-	-	-
1	5.8582(4)	14.2571(10)	423.7(5)	5.8580(2)	14.2605(9)	423.8(2)
2	5.8879(5)	14.3067(13)	429.5(6)	5.8959(1)	14.3274(7)	431.3(7)
3	5.9097(4)	14.3315(11)	433.5(5)	5.9215(1)	14.3627(9)	436.1(9)

Table S3: Refined lattice parameters for $KMgH_xF_{3-x}$ are used in Fig. 5.

x	$KMgH_xF_{3-x}$ (X-ray data)	
	a [Å]	V [Å3]
0	3.9854(1)	63.3
1	3.9948(1)	63.8
2	4.0137(1)	64.7
3	4.0252(1)	65.2

Table S4. Refined lattice parameters and atomic parameters for $KMgD_2F$. Lattice parameters from high-resolution neutron data; atomic parameters and occupancy parameters from simultaneous refinement of X-ray and neutron data.

$KMgD_2F$		*a* = 4.0078(3) Å, *V* = 64.4(9) Å^3				
Atom	Site	x	y	z	B_{iso}(Å^2)	s.o.f.
K1	1*b*	1/2	1/2	1/2	0.290(7)	1
Mg1	1*a*	0	0	0	0.013(2)	1
D1/F1	3*d*	1/2	0	0	1.080(14)	0.64(8) D / 0.36(8) F