

**Electronic Supporting Information**

**Probing the Site-Selective Doping and Charge Compensating Defects in  
KMgF<sub>3</sub>: Insights from a Hybrid DFT Study**

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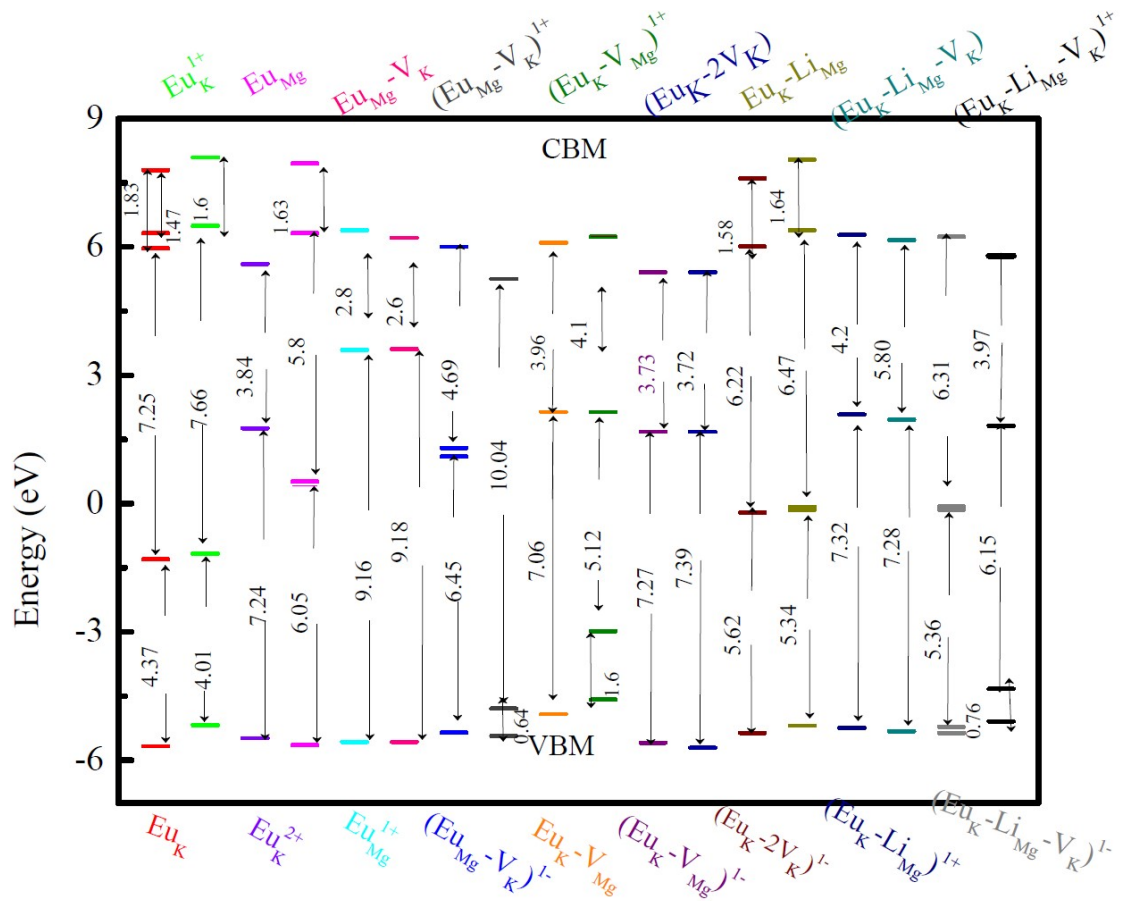
**Table S1: Variation of Structural Parameter for Eu-doped KMgF<sub>3</sub> using 3 × 3 × 3 supercell**

System	Cell Parameter (Å)	Cell Volume (Å <sup>3</sup> )	d <sub>Mg-F</sub> (Å)	d <sub>K-F</sub> (Å)	d <sub>Eu-F</sub> (Å)	d <sub>Li-F</sub> (Å)
KMgF <sub>3</sub>	12.08	1764	2.01	2.85	--	--
Eu <sub>K</sub> -KMgF <sub>3</sub>	12.10	1772	1.99-2.03	2.82-2.88	2.74	--
Eu <sub>K</sub> <sup>1+</sup> -KMgF <sub>3</sub>	12.05	1749	1.98-2.02	2.81-2.87	2.73	--
Eu <sub>K</sub> <sup>2+</sup> -KMgF <sub>3</sub>	12.01	1733	1.97-2.03	2.81-2.87	2.58	--
Eu <sub>Mg</sub> -KMgF <sub>3</sub>	12.13	1785	1.88-2.04	2.80-2.93	2.26	--
Eu <sub>Mg</sub> <sup>1+</sup> -KMgF <sub>3</sub>	12.09	1768	1.93-2.02	2.72-2.97	2.17	--
Eu <sub>K</sub> +V <sub>Mg</sub> -KMgF <sub>3</sub>	12.08	1762	1.94-2.05	2.78-2.87	2.23	--
(Eu <sub>K</sub> +V <sub>Mg</sub> ) <sup>1+</sup> -KMgF <sub>3</sub>	12.10	1774	1.97-2.05	2.82-2.87	2.23	--
(Eu <sub>K</sub> +V <sub>Mg</sub> ) <sup>1-</sup> -KMgF <sub>3</sub>	12.15	1795	1.95-2.06	2.81-2.89	2.26	--
(Eu <sub>K</sub> +2V <sub>K</sub> )-KMgF <sub>3</sub>	12.04	1745	1.96-2.05	2.81-3.09	2.56	--
(Eu <sub>K</sub> +2V <sub>K</sub> ) <sup>1+</sup> -KMgF <sub>3</sub>	12.03	1739	1.96-2.05	2.80-3.09	2.46	--
(Eu <sub>K</sub> +2V <sub>K</sub> ) <sup>1-</sup> -KMgF <sub>3</sub>	12.14	1789	2.00-2.03	2.83-3.04	2.59	--
(Eu <sub>Mg</sub> -V <sub>K</sub> )-KMgF <sub>3</sub>	12.12	1781	1.94-2.05	2.83-2.93	2.20	--
(Eu <sub>Mg</sub> -V <sub>K</sub> ) <sup>1+</sup> -KMgF <sub>3</sub>	12.11	1774	1.94-2.05	2.81-2.89	2.19	--
(Eu <sub>Mg</sub> -V <sub>K</sub> ) <sup>1-</sup> -KMgF <sub>3</sub>	12.17	1802	1.95-2.07	2.81-2.82	2.18	--
Eu <sub>K</sub> -Li <sub>Mg</sub>	12.08	1762	1.98-2.01	2.76-2.86	2.37	1.96

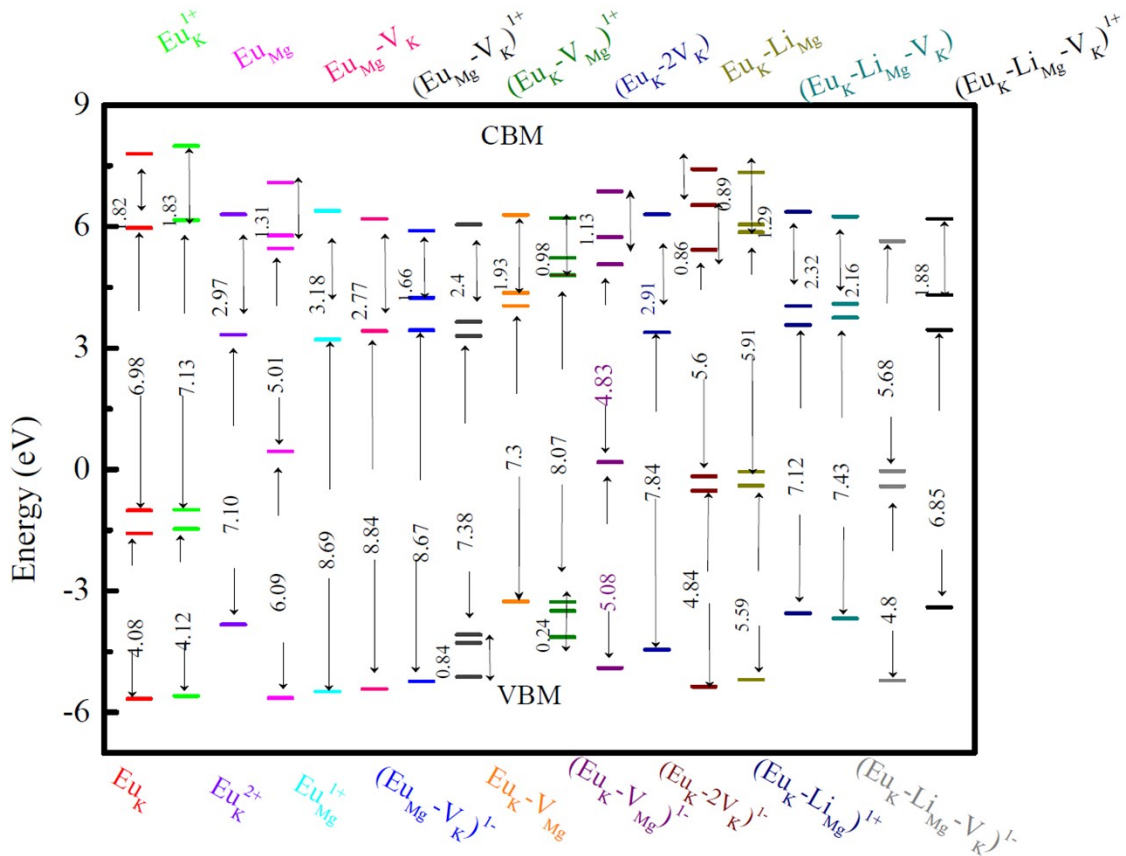
			2.03	3.02		
$(\text{Eu}_K\text{-Li}_{\text{Mg}})^{1+}$	12.05	1747	1.96 2.00 2.04	3.09 2.85 2.77	2.63 2.32	1.93 2.21
$\text{Eu}_K\text{-Li}_{\text{Mg}}\text{-V}_K$	12.06	1753	1.97 2.00 2.03	2.77 2.87 2.89	2.48 2.75	1.95 2.18
$(\text{Eu}_K\text{-Li}_{\text{Mg}}\text{-V}_K)^{1+}$	12.03	1741	1.97 2.00 2.03	2.77 2.87 3.10	2.37 2.46 2.75	1.96 2.13
$(\text{Eu}_K\text{-Li}_{\text{Mg}}\text{-V}_K)^{1-}$	12.09	1768	1.99 2.04	2.83 2.86 3.07	2.38 2.60 2.74	1.97 2.19
$\text{Eu}_{\text{Mg}}\text{-Li}_K$	12.13	1785	1.94 2.02 2.06	2.85 2.28	2.17 2.28	2.10
$(\text{Eu}_{\text{Mg}}\text{-Li}_K)^{1+}$	12.11	1775	1.94 2.00 2.05	2.85- 2.87	2.15- 2.18	1.95
$(\text{Eu}_{\text{Mg}}\text{-Li}_K)^{1-}$	12.17	1803	1.95 2.05	2.82- 2.87	2.18- 2.35	2.22

**Table S2: Variation of Bader Charge on the Eu-Center**

System	Bader Charge
KMgF <sub>3</sub>	--
Eu <sub>K</sub> -KMgF <sub>3</sub>	1.66
Eu <sub>K</sub> <sup>1+</sup> -KMgF <sub>3</sub>	1.68
Eu <sub>K</sub> <sup>2+</sup> -KMgF <sub>3</sub>	2.21
Eu <sub>Mg</sub> -KMgF <sub>3</sub>	1.67
Eu <sub>Mg</sub> <sup>1+</sup> -KMgF <sub>3</sub>	2.16
Eu <sub>K</sub> +V <sub>Mg</sub> <sup>-</sup> - KMgF <sub>3</sub>	2.16
(Eu <sub>K</sub> +V <sub>Mg</sub> ) <sup>1+</sup> - KMgF <sub>3</sub>	2.18
(Eu <sub>K</sub> +V <sub>Mg</sub> ) <sup>1-</sup> - KMgF <sub>3</sub>	1.68
(Eu <sub>K</sub> +2V <sub>K</sub> ) <sup>-</sup> - KMgF <sub>3</sub>	2.21
(Eu <sub>K</sub> +2V <sub>K</sub> ) <sup>1+</sup> - KMgF <sub>3</sub>	2.27
(Eu <sub>K</sub> +2V <sub>K</sub> ) <sup>1-</sup> - KMgF <sub>3</sub>	1.70
(Eu <sub>Mg</sub> -V <sub>K</sub> )-KMgF <sub>3</sub>	2.15
(Eu <sub>Mg</sub> -V <sub>K</sub> ) <sup>1+</sup> KMgF <sub>3</sub>	2.27
(Eu <sub>Mg</sub> -V <sub>K</sub> ) <sup>1-</sup> KMgF <sub>3</sub>	1.70
Eu <sub>K</sub> -Li <sub>Mg</sub>	1.66
(Eu <sub>K</sub> -Li <sub>Mg</sub> ) <sup>1+</sup>	2.18
Eu <sub>K</sub> -Li <sub>Mg</sub> -V <sub>K</sub>	2.19
(Eu <sub>K</sub> -Li <sub>Mg</sub> -V <sub>K</sub> ) <sup>1+</sup>	2.26
(Eu <sub>K</sub> -Li <sub>Mg</sub> -V <sub>K</sub> ) <sup>1-</sup>	1.67
Eu <sub>Mg</sub> -Li <sub>K</sub>	1.67
(Eu <sub>Mg</sub> -Li <sub>K</sub> ) <sup>1+</sup>	2.14
(Eu <sub>Mg</sub> -Li <sub>K</sub> ) <sup>1-</sup>	1.57



**Fig. S1: Alignment of different energy levels for Eu-doped KMgF<sub>3</sub> in the presence of different defects.**



**Fig. S2: Alignment of different energy levels for Eu-doped KMgF<sub>3</sub> in the presence of different defects including spin-orbit coupling.**