

# Theoretical study of the phase transformations of $\text{Sr}_3\text{Hf}_2\text{O}_7$

E. Lora da Silva<sup>1\*</sup>, A. Mokhles Gerami<sup>2,3</sup>, P. Neenu Lekshmi,<sup>1</sup> J. G. M. Correia,<sup>4,3</sup> J. P. Araujo,<sup>1</sup> A. M. L Lopes<sup>1</sup>

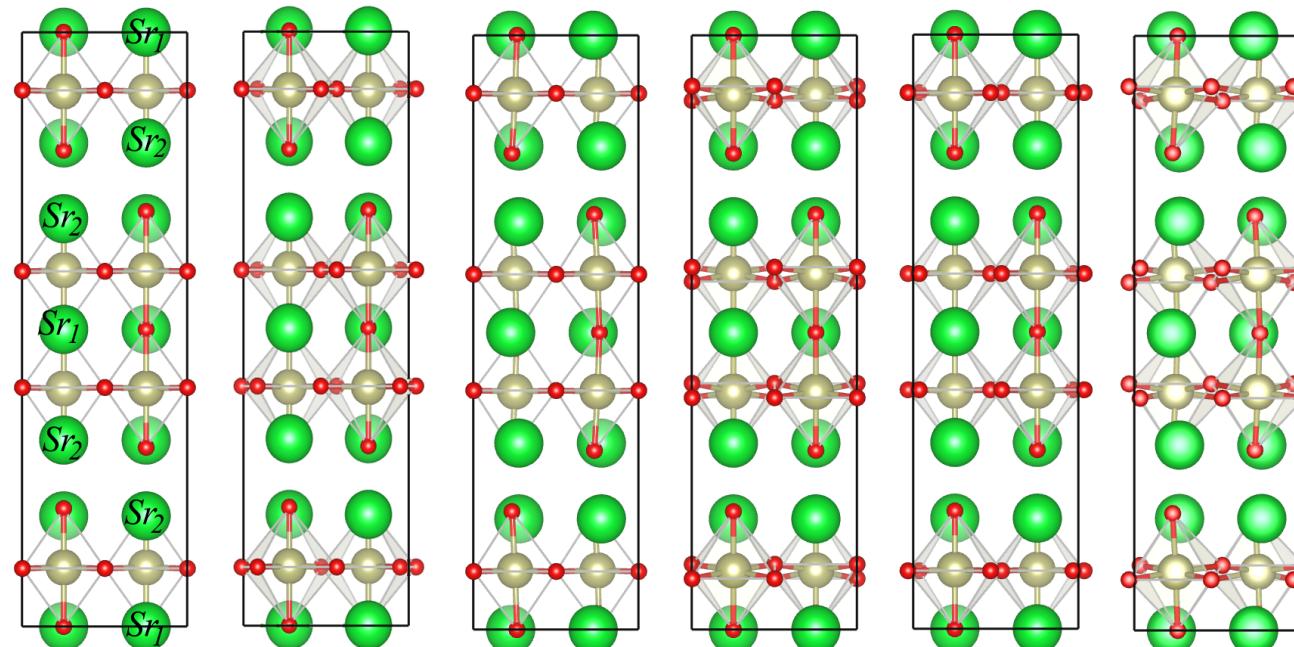
<sup>1</sup> IFIMUP, Depart. Physics and Astronomy, Faculty of Sciences, University of Porto,

<sup>2</sup>School of Particles and Accelerators, Institute for Research in Fundamental Sciences

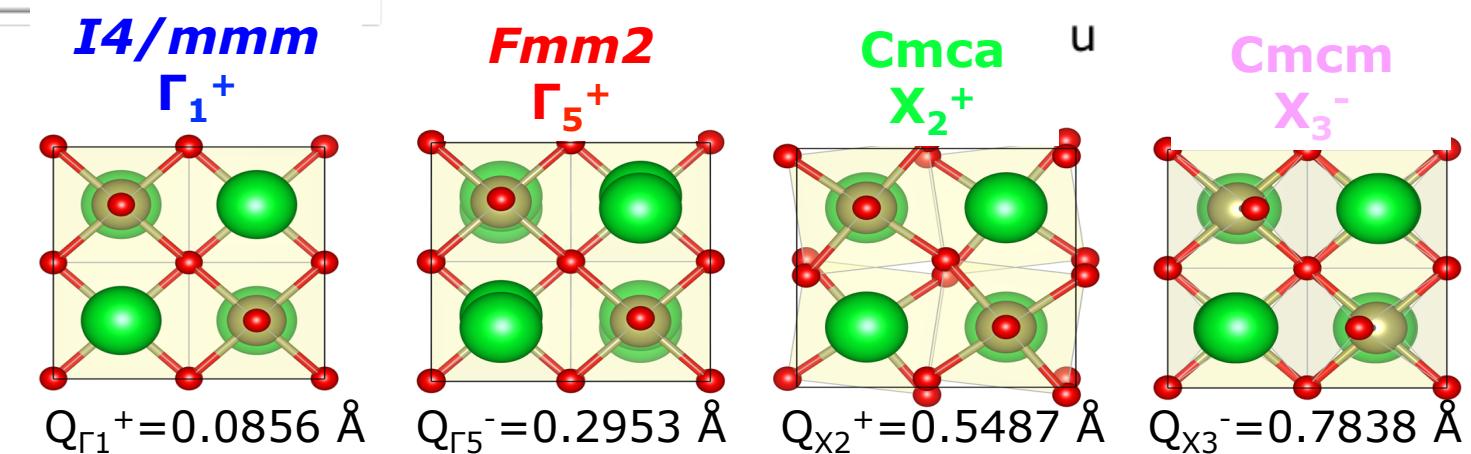
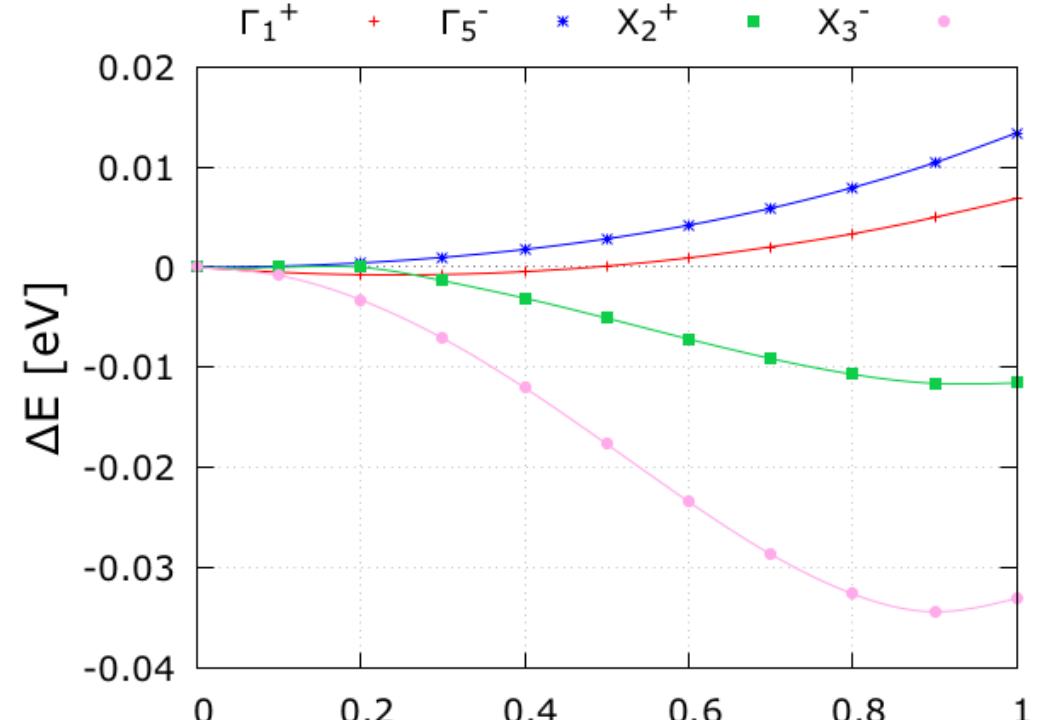
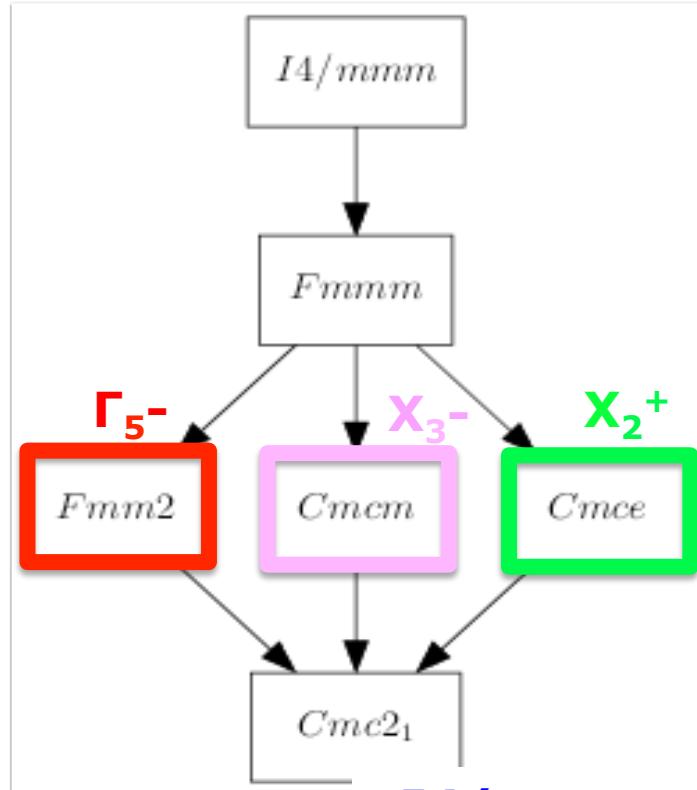
<sup>3</sup>CERN, Esplanade des Particules 1, Geneva 23

<sup>4</sup>C2TN, Depart. Eng. Ciências Nucleares, IST, Universidade de Lisboa

$I4/mmm$	$Ccce$	$Fmm2$	$Cmcm$	$Cmca$	$Cmc2_1$
S.G.139	S.G.68	S.G.42	S.G.63	S.G.64	S.G.36

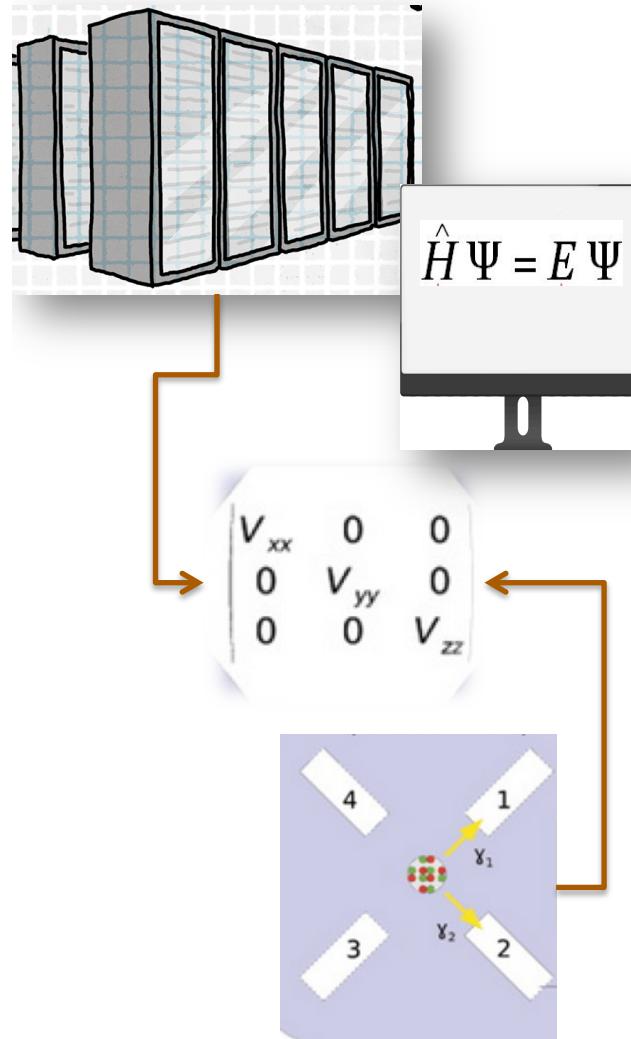


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Calculated electric field gradients ( $V_{zz}$ ) and asymmetric parameter ( $\eta$ )



Space Group	$\text{Sr}_1$		$\text{Sr}_2$		$\text{Hf}$	
	$V_{zz}$ (V/ $\text{\AA}^2$ )	$\eta$	$V_{zz}$ (V/ $\text{\AA}^2$ )	$\eta$	$V_{zz}$ (V/ $\text{\AA}^2$ )	$\eta$
<i>I4/mmm</i>	11.84	0.000	-77.91	0.000	16.38	0.000
<i>Ccce</i>	-58.21	0.001	-90.77	0.672	72.37	0.010
<i>Fmm2</i>	11.60	0.011	-76.44	0.000	20.15	0.037
<i>Cmcm</i>	-41.54	0.724	-54.48	0.769	48.87	0.701
<i>Cmca</i>	74.21	0.163	-119.55	0.606	-89.63	0.129
<i>Cmc2<sub>1</sub></i>	-43.79	0.731	-58.31	0.955	37.18	0.408

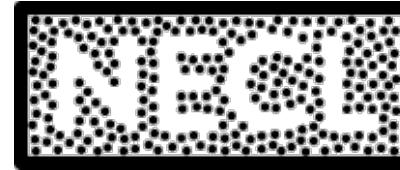
# Acknowledgments



**IFIMUP**

Instituto de Física de  
Materiais Avançados,  
Nanotecnologia e Fotónica

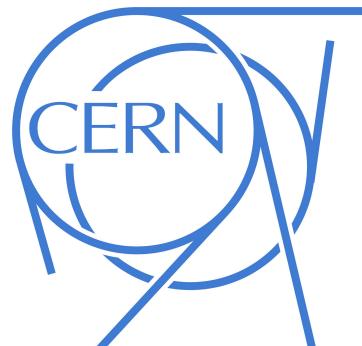
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