Electron-Phonon Coupling in Luminescent Europium-Doped Hydride Perovskites Studied by Luminescence Spectroscopy, Inelastic Neutron Scattering, and First-Principles Calculations

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Table 1: Wyckoff sites for the inverse cubic perovskite structure type of $LiMH_3$ or $LiMD_3$ (M = Sr, Ba), space group $Pm\bar{3}m$.

site	site sym.	atom	x	y	z	occ.
$1a$	$m\bar{3}m$	Li	0	0	0	1
$1b$	$m\bar{3}m$	M	1/2	1/2	1/2	1
$3d$	$m\bar{3}m$	H/D	1/2	0	0	1

Table 2: Refined lattice parameters and interatomic distances (in pm) in $LiMH_3$:Eu^{2+} and $LiMD_3$:Eu^{2+}, Eu^{2+} 0.005% or 0%, respectively (M = Sr, Ba), space group $Pm\bar{3}m$, X-ray data were collected on a STOE Stadi P powder diffractometer (Stoe & Cie GmbH) with $CuK_{\alpha 1}$ radiation or a Huber G670 diffractometer with Guinier geometry at T = 297(2) K with $CuK_{\alpha 1}$ radiation, as well as amount of side product MH_2 or MD_2 in w%. Estimated standard deviations provided by the program TOPAS are given in parenthesis. Calculated values for comparison (Vienna Ab Initio Program Package).

$LiSrH_3$:Eu^{2+}	(0.005 mol%)	a = 383.461(2)
Eu/Sr – H	271.148(2)	
Li – H	191.731(2)	SrH_2 0 w%
$LiSrD_3$:Eu^{2+}	(0.005 mol%)	a = 381.765(2)
Eu/Sr – D	269.948(2)	
Li – D	190.882(2)	SrD_2 0 w%
$LiBaH_3$:Eu^{2+}	(0.005 mol%)	a = 402.526(7)
Eu/Ba – H	284.629(4)	
Li – H	201.263(4)	BaH_2 8.8(9) w%
$LiBaD_3$:Eu^{2+}	(0.005 mol%)	a = 400.870(2)
Eu/Ba – D	283.458(2)	
Li – D	200.435(2)	BaD_2 0 w%
$LiSrH_3$	a = 382.475(17)	
Sr – H	270.451(12)	
Li – H	191.238(9)	SrH_2 25.2 w%
$LiBaH_3$	a = 401.370(3)	
Ba – H	283.811(2)	
Li – H	200.069(2)	BaH_2 27.6 w%
$LiBaD_3$	a = 400.840(4)	
Ba – D	283.437(3)	
Li – D	200.420(2)	BaD_2 48.2 w%
Calculated values (VASP)		
$LiSrH_3$	a = 380.8	
Sr – H	269.3	
Li – H	190.4	
$LiSrD_3$	a = 380.8	
Sr – D	269.3	
Li – D	190.4	
$LiBaH_3$	a = 402.0	
Ba – H	284.3	
Li – H	201.0	
$LiBaD_3$	a = 402.0	
Ba – D	284.3	
Li – D	201.0	

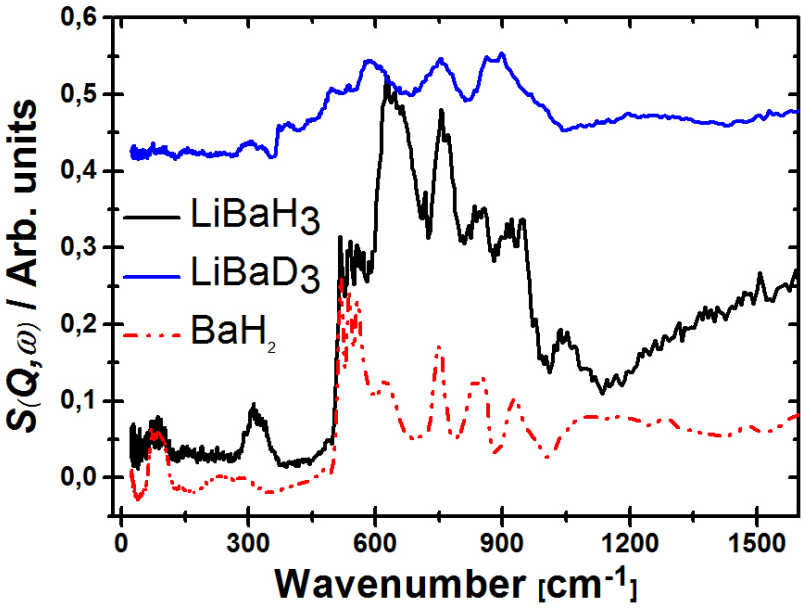

Figure 1: Frequency distributions for $LiBaH_3$ and $LiBaD_3$ as measured and BaH_2 for comparison. Recorded at TOSCA at 20 K.

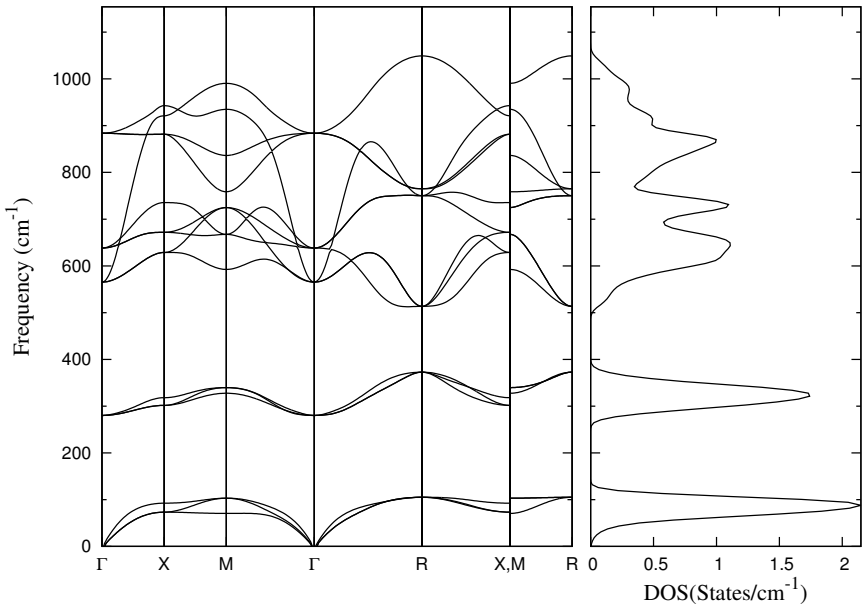

Figure 2: Phonon dispersion and density of states of $LiBaH_3$ as calculated by using the VASP program package.

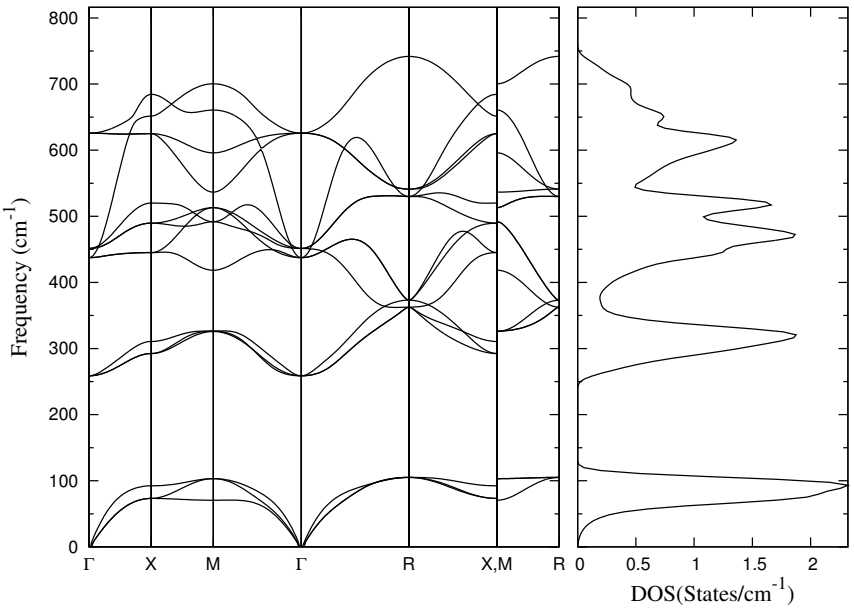

Figure 3: Phonon dispersion and density of states of $LiBaD_3$ as calculated by using the VASP program package.

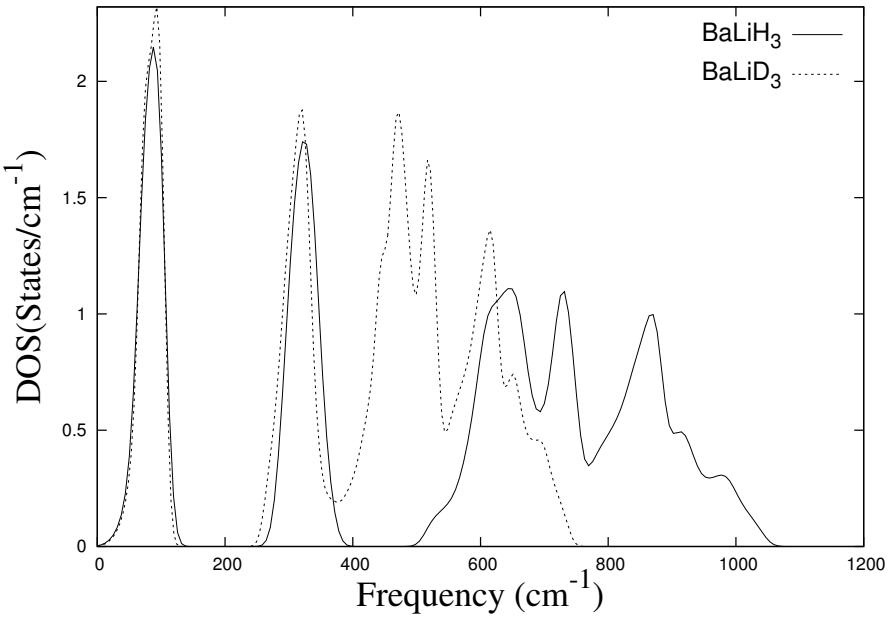

Figure 4: Comparison of the phonon densities of states of the hydride $LiBaH_3$ and the deuteride $LiBaD_3$ as calculated by using the VASP program package.