Supplementary Materials

Electronic structure calculation of Cr^{3+} and Fe^{3+} in phosphor host materials based on relaxed structures by molecular dynamics simulation

Joichiro Ichikawa[1], Hiroko Kominami[2], Kazuhiko Hara[3], Masato Kakihana[4] and Yuta Matsushima[1,*]

[1] Chemistry and Chemical Engineering, Yamagata University, Yamagata 992-8510, Japan;
[2] Electronics and Materials Science, Shizuoka University, Shizuoka 432-8561, Japan; kominami.hiroko@shizuoka.ac.jp
[3] Research Institute of Electronics, Shizuoka University, Shizuoka 432-8011, Japan; hara.kazuhiko@shizuoka.ac.jp
[4] Institute of Scientific and Industrial Research, Osaka University, Osaka 567-0047, Japan; kakihana@sanken.osaka-u.ac.jp
* Correspondence: ymatsush@yz.yamagata-u.ac.jp; Tel.: +81-238-26-3165

Table S1. Comparison of the lattice parameters simulated by MD using the potential parameters (A_{ij} and ρ_{ij}) in **Table 1** with those experimentally determined (Exp.). MSD represents the "mean square displacement" in MD.

Figure S1. Crystal structures of (a) $LiAl_5O_8$, (b) α-Al_2O_3, and (c) γ-$LiAlO_2$.

Figure S2. Emission and excitation spectra of (a) $LiAl_5O_8:Cr^{3+}$, (b) α-$Al_2O_3:Cr^{3+}$, and (c) γ-$LiAlO_2:Fe^{3+}$.

Figure S3. Calculation clusters for isolated Cr^{3+} and Fe^{3+} in (a) $LiAl_5O_8:Cr^{3+}$ [$(Li_2Al_{10}CrO_{38})^{41-}$], (b) α-$Al_2O_3:Cr^{3+}$ [$(Al_{13}CrO_{45})^{48-}$], and (c) γ-$LiAlO_2:Fe^{3+}$ [$(Li_9Al_6FeO_{32})^{34-}$].

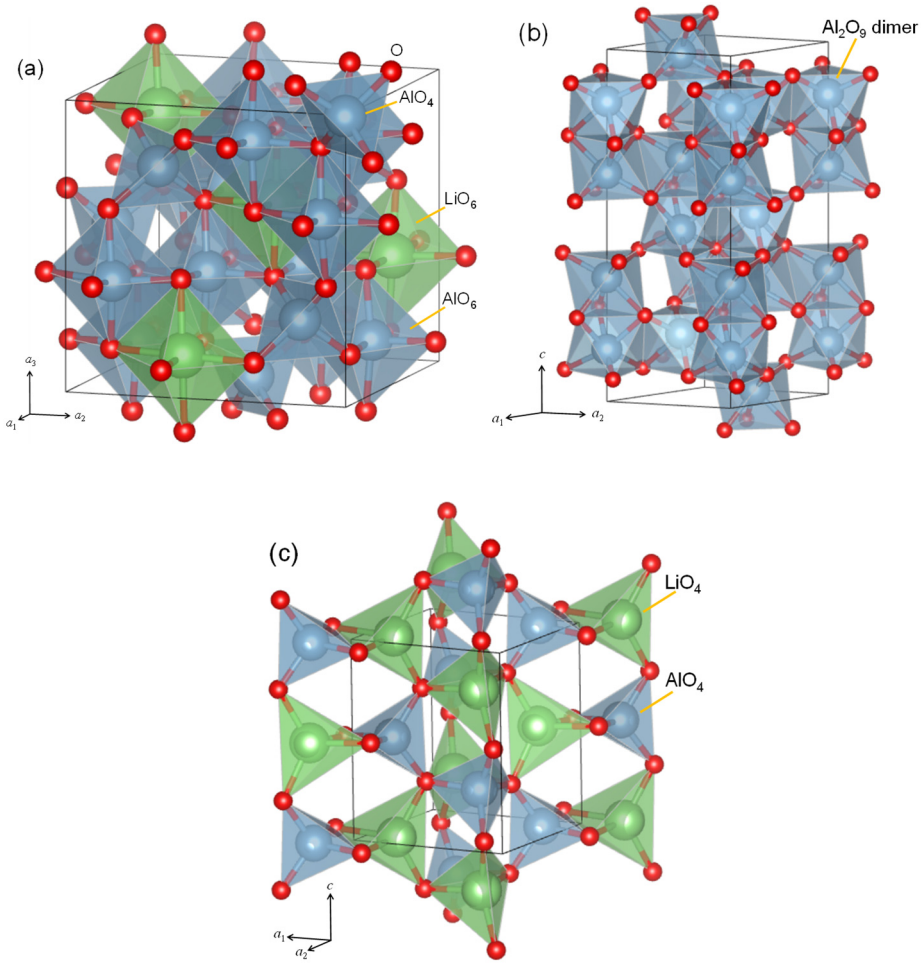
Figure S4. The clusters for the calculation of the electronic interaction in the Fe–Fe pairs on (a) first-, (b) second-, and (c) third-nearest cation sites.

*The crystal structures in **Figure S1** and the calculation clusters in **Figure S3** and **S4** are illustrated by VESTA [*i*].

i Momma, K.; Izumi, F. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. *J. Appl. Crystallogr.* **2011**, *44*, 1272-1276.

Table S1 Comparison of the lattice parameters simulated by MD using the potential parameters (A_{ij} and ρ_{ij}) in **Table 1** with those experimentally determined (Exp.). MSD represents the "mean square displacement" in MD.

Material	Method	Lattice parameter (Å) *The values in parentheses in the MD rows are difference (%) between Exp. and MD.			MSD (Å^2)	Ref.
		a	*b*	*c*		
α-Al_2O_3	Exp.	4.7540	4.7540	12.990	–	21
	MD	4.76 (+0.13%)	4.75 (−0.08%)	12.87 (−0.92%)	Al: 0.012 O: 0.006	–
Li_2O	Exp.	4.610	4.610	4.610	–	24
	MD	4.67 (+1.30%)	4.67 (+1.30%)	4.67 (+1.30%)	Li: 0.025 O: 0.013	–
α-$LiAlO_2$	Exp.	2.8003	2.8003	14.216	–	25
	MD	2.85 (+1.77%)	2.85 (+1.77%)	14.48 (+1.86%)	Al: 0.008 Li: 0.029 O: 0.015	–
γ-$LiAlO_2$	Exp.	5.1687	5.1687	6.2679	–	22
	MD	5.23 (+1.19%)	5.23 (+1.19%)	6.22 (−0.76%)	Al: 0.007 Li: 0.032 O: 0.037	–
$LiAl_5O_8$	Exp.	7.908	7.908	7.908	–	20
	MD	7.87 (−0.48%)	7.87 (−0.48%)	7.87 (−0.48%)	Al: 0.006 Li: 0.011 O: 0.010	–
Cr_2O_3	Exp.	4.9507	4.9507	13.5656	–	26
	MD	4.94 (−0.22%)	4.94 (−0.22%)	13.37 (−1.44%)	Cr: 0.034 O: 0.008	–
$LiCrO_2$	Exp.	2.9010	2.9010	14.4311	–	27
	MD	2.95 (+1.69%)	2.95 (+1.69%)	14.62 (+1.31%)	Cr: 0.006 Li: 0.029 O: 0.031	–
Fe_2O_3	Exp.	5.0355	5.0355	13.7471	–	28
	MD	5.01 (−0.51%)	5.02 (−0.31%)	13.49 (−1.87%)	Fe: 0.013 O: 0.009	–
$LiFe_5O_8$	Exp.	8.319	8.319	8.319	–	29
	MD	8.25 (−0.83%)	8.25 (−0.83%)	8.25 (−0.83%)	Fe: 0.018 Li: 0.023 O: 0.036	–



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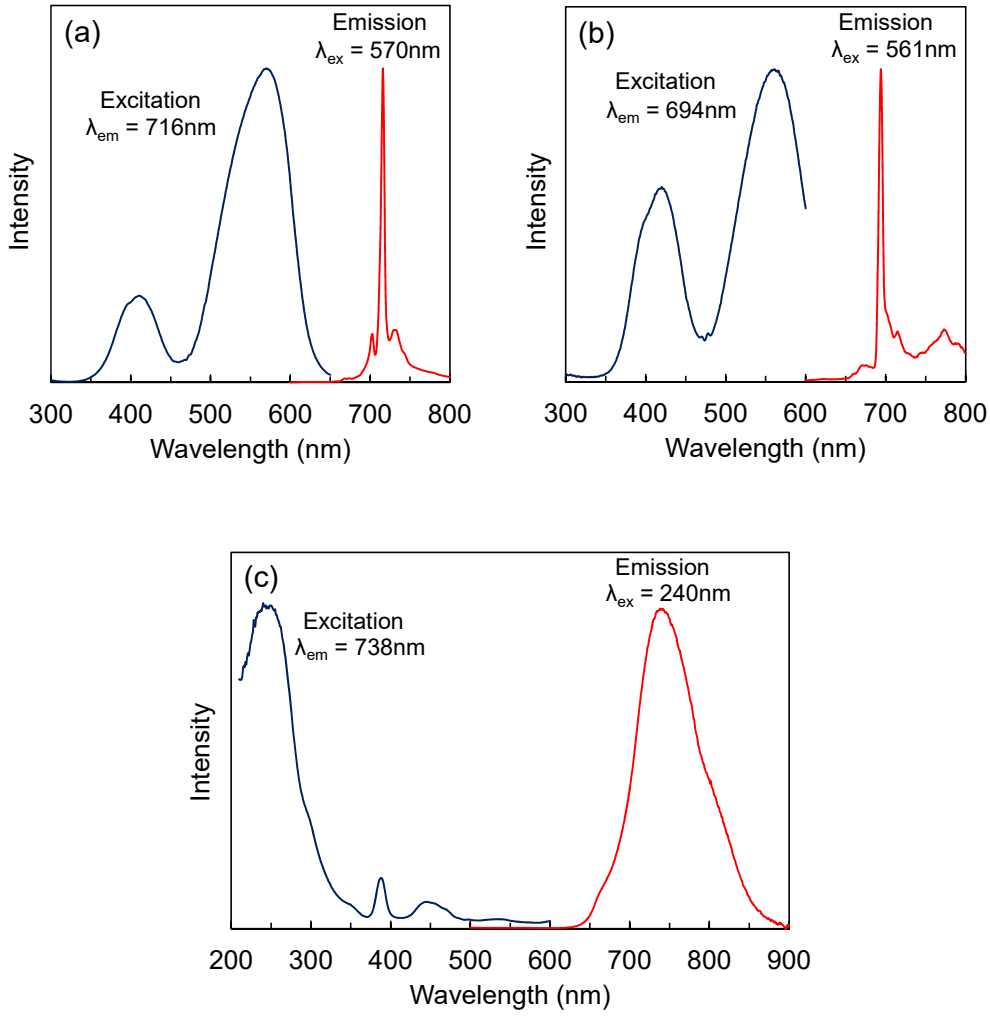

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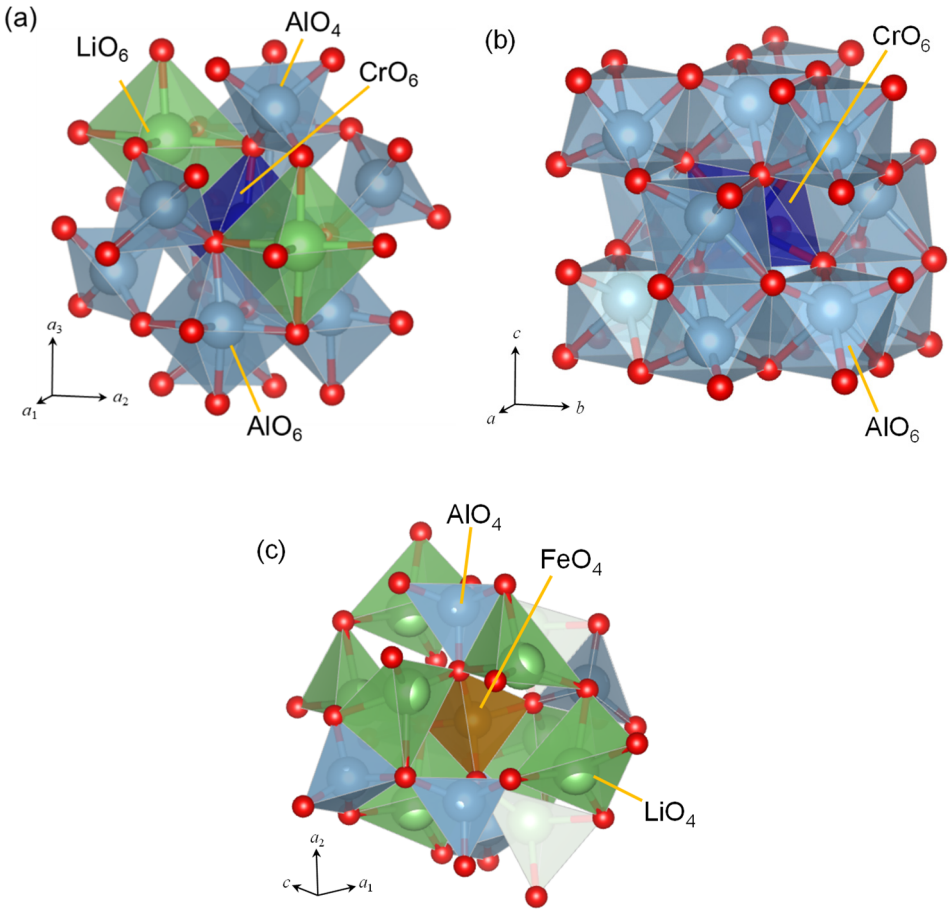

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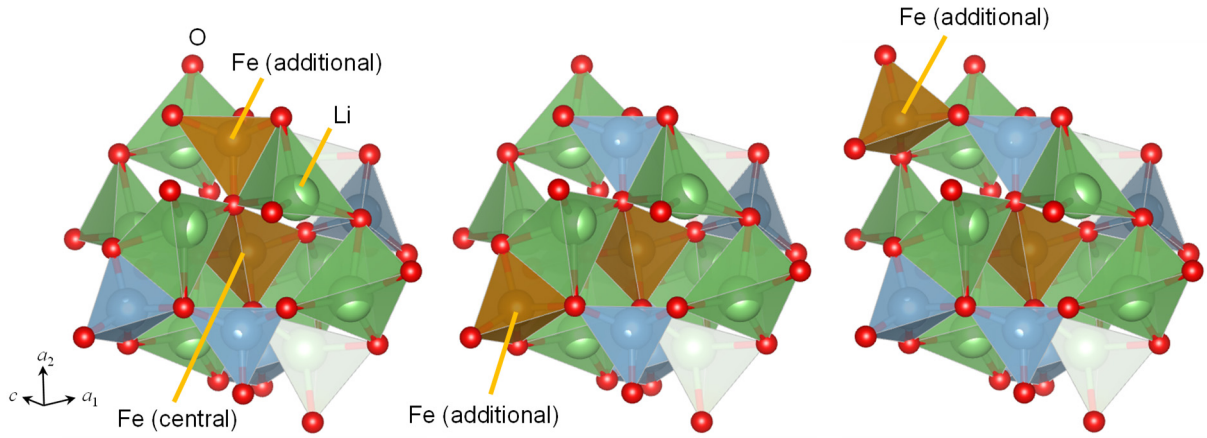

(a) First nearest (b) Second nearest (c) Third nearest

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