

Supplementary Information

NASICON-type $\text{Na}_{3.6}\text{Lu}_{1.8-x}(\text{PO}_4)_3:x\text{Eu}^{3+}$ phosphors: structure and luminescence

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Table S1. Element analysis results of $\text{Na}_{3.6}\text{Lu}_{1.8-x}(\text{PO}_4)_3:x\text{Eu}^{3+}$ ($x = 0, 0.3$).

| NLPO: $x\text{Eu}$ | P, at. % | Lu, at. % | Eu, at. % | P:Lu:Eu ratio |
|--------------------|------------------|------------------|-----------------|-------------------|
| $x = 0$ | 63.81 ± 0.45 | 36.19 ± 0.45 | - | 3:1.70(3):0 |
| $x = 0.30$ | 62.99 ± 0.57 | 31.07 ± 0.35 | 5.94 ± 0.23 | 3:1.48(4):0.28(2) |

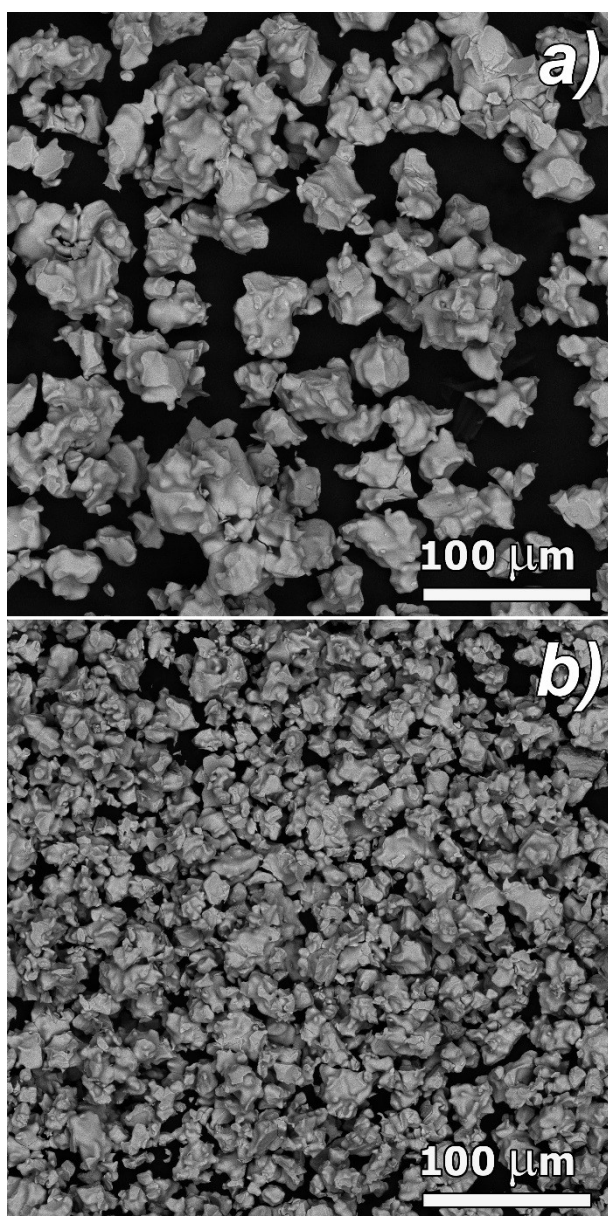


Figure S1. SEM images of $\text{Na}_{3.6}\text{Lu}_{1.8-x}(\text{PO}_4)_3:x\text{Eu}^{3+}$ ($x = 0$ (a), 0.3 (b)).

Table S2. The unit cell parameters for Na_{3.6}Lu_{1.8-x}(PO₄)₃:xEu³⁺.

| <i>x</i> | <i>a</i> , Å | <i>c</i> , Å | <i>V</i> , Å ³ |
|----------|--------------|--------------|---------------------------|
| 0.05 | 9.1050(2) | 22.2467(6) | 1597.17(6) |
| 0.1 | 9.1080(3) | 22.2086(1) | 1595.51(7) |
| 0.3 | 9.1176(2) | 22.1982(7) | 1598.12(7) |
| 0.4 | 9.1208(2) | 22.1803(6) | 1597.94(6) |
| 0.45 | 9.1216(1) | 22.1409(4) | 1595.39(5) |
| 0.5 | 9.1259(2) | 22.1473(8) | 1597.37(8) |
| 0.6 | 9.1263(2) | 22.1375(8) | 1596.80(8) |
| 0.7 | 9.1335(1) | 22.1481(9) | 1600.08(5) |

Table S3. Atomic coordinates, isotropic displacement atomic parameters (*U*_{iso}), site occupation of Na_{3.6}Lu_{1.8}(PO₄)₃ and anisotropic temperature factors (*U*_{ij} in Å²) of the Lu site.

| Position | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> _{iso} *100, Å ² | Occupancy | |
|----------|------------------------|------------------------|------------------------|--|--------------------------|------------------------|
| Lu | 0 | 0 | 0.15551(8) | 1.22(5) | 0.950(9)Lu | |
| Na4 | 0 | 0 | 0.15551(8) | 0.00(1) | 0.050(9)Na | |
| Na1 | 0.138(3) | 0.077(5) | 0.0232(10) | 0.26(12) | 0.268(11)Na ⁺ | |
| Na2 | 0.6655(16) | 0 | 0.25 | 0.32(9) | 0.453(8)Na ⁺ | |
| Na3 | 0 | 0 | 0.25 | 0.9(2) | 0.53(3)Na ⁺ | |
| P1 | 0.2959(7) | 0 | 0.25 | 0.9(2) | 1P | |
| O1 | 0.214(1) | -0.0207(9) | 0.1825(5) | 0.7(2) | 1O | |
| O2 | 0.1996(10) | 0.1762(11) | 0.0966(5) | 0.7(2) | 1O | |
| | <i>U</i> ¹¹ | <i>U</i> ²² | <i>U</i> ³³ | <i>U</i> ¹² | <i>U</i> ¹³ | <i>U</i> ²³ |
| Lu | 0.0023(5) | 0.0023(5) | 0.032(1) | 0.0011(3) | 0 | 0 |

Table S4. Selected bond lengths (Å) and angles (°) for Na_{3.6}Lu_{1.8}(PO₄)₃.

| Polyhedron | Distance | <i>d</i> , Å | Polyhedron | Distance | <i>d</i> , Å |
|-------------------------|----------|--------------|-------------------------|-----------------------|--------------|
| Na1O₆ | Na1-O1 | 2.46(6) | Na2O₈ | Na2-O1×2 | 2.428(4) |
| | Na1-O1 | 3.06(5) | | Na2-O1×2 | 2.946(9) |
| | Na1-O2 | 1.82(3) | | Na2-O2×2 | 2.472(11) |
| | Na1-O2 | 2.74(4) | | Na2-O2×2 | 2.828(18) |
| | Na1-O2 | 2.91(3) | | <Na2-O> | 2.669 |
| | Na1-O2 | 3.12(3) | | PO₄ | P-O1×2 |
| <Na1-O> | 2.69 | P-O1×2 | 1.529(8) | | |
| | | <P-O> | 1.590 | | |

| (Lu/Na4)O₆ - octahedron | | | | | | |
|---|-----------|-----------|-----------|----------|----------|----------|
| Lu/Na4 | O1 | O1 | O1 | O2 | O2 | O2 |
| O1 | 2.1372(5) | 112.40(4) | 112.40(4) | 76.8(3) | 78.9(3) | 158.9(3) |
| O1 | | 2.1372(5) | 112.40(4) | 78.9(3) | 158.9(3) | 76.8(3) |
| O1 | | | 2.1372(5) | 158.9(3) | 76.8(3) | 78.9(3) |
| O2 | | | | 2.166(9) | 87.0(4) | 87.0(4) |
| O2 | | | | | 2.166(9) | 87.0(4) |
| O2 | | | | | | 2.166(9) |
| <(Lu/Na4)- >O> | 2.1516 | | | | | |

| Na3O₆- polyhedron | | | | | | |
|-------------------------------------|----------|----------|----------|----------|----------|----------|
| Na3 | O1 | O1 | O1 | O1 | O1 | O1 |
| O1 | 2.545(3) | 88.5(3) | 88.5(3) | 73.14(4) | 125.6(4) | 139.5(4) |
| O1 | | 2.545(3) | 88.5(3) | 139.5(4) | 73.14(4) | 125.6(4) |
| O1 | | | 2.545(3) | 125.6(4) | 139.5(4) | 73.14(4) |
| O1 | | | | 2.545(3) | 88.5(3) | 88.5(3) |
| O1 | | | | | 2.545(3) | 88.5(3) |
| O1 | | | | | | 2.545(3) |

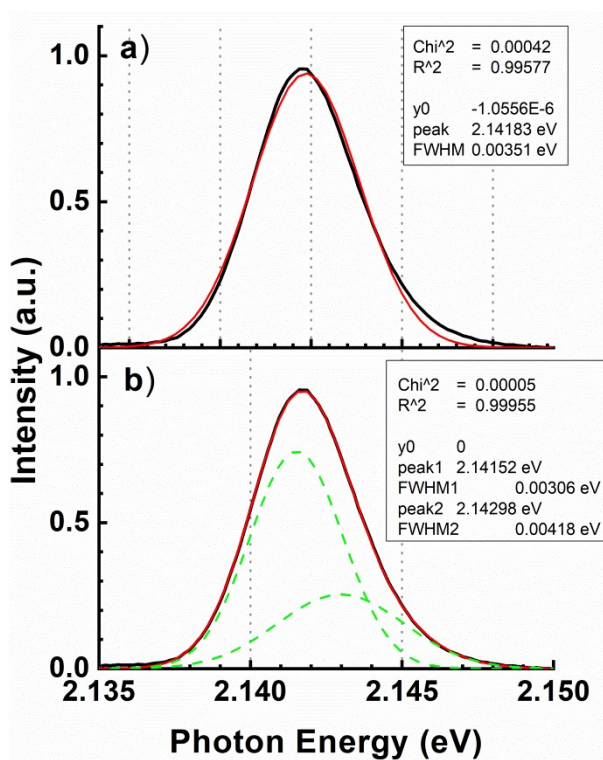


Figure S2. Fitting of the peak 2.141 eV (579 nm, $^5D_0 \rightarrow ^7F_0$ transitions) of $\text{Na}_{3.6}\text{Lu}_{1.3}(\text{PO}_4)_3:0.5\text{Eu}^{3+}$ with single (a) and two (b) Gaussian functions.