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# Local Environment Rigidity and the Evolution of Optical Properties in the Green-Emitting Phosphor $Ba_{1-x}Sr_xScO_2F:Eu^{2+}$

## Supporting Information

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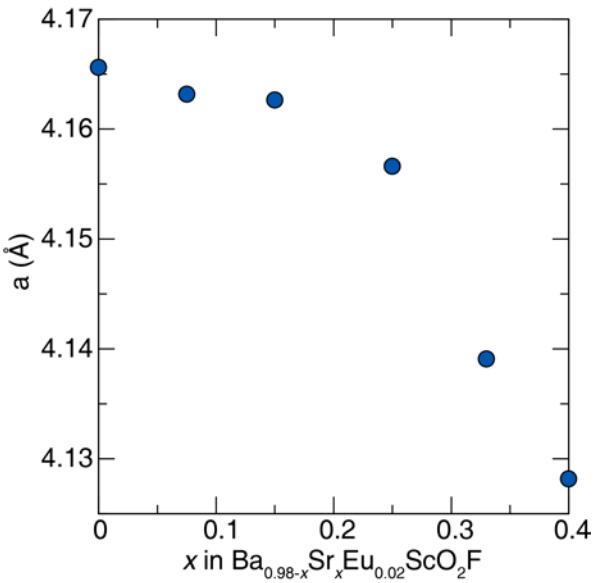


**Figure S1.** Le Bail refinements of $(Ba_{1-x}Sr_x)_{0.98}Eu_{0.02}ScO_2F$ ($x$ = 0.075, 0.15, 0.25, 0.33, 0.40) show that the lattice parameters decrease following Vegard's law.

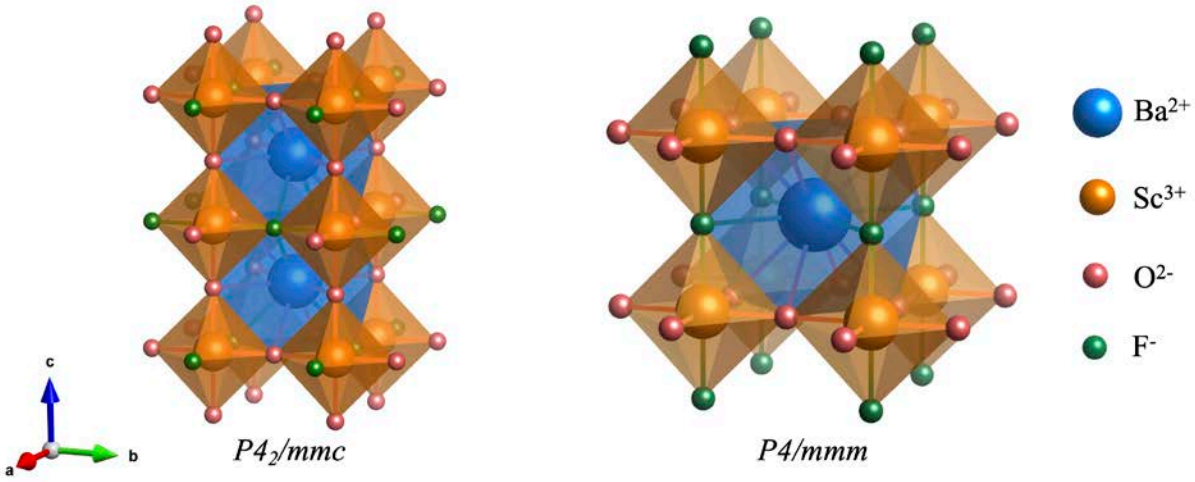


**Figure S2.** The recovered DFT ordered phases of $BaScO_2F$ of *P4₂/mmc* and *P4/mmm* space groups.

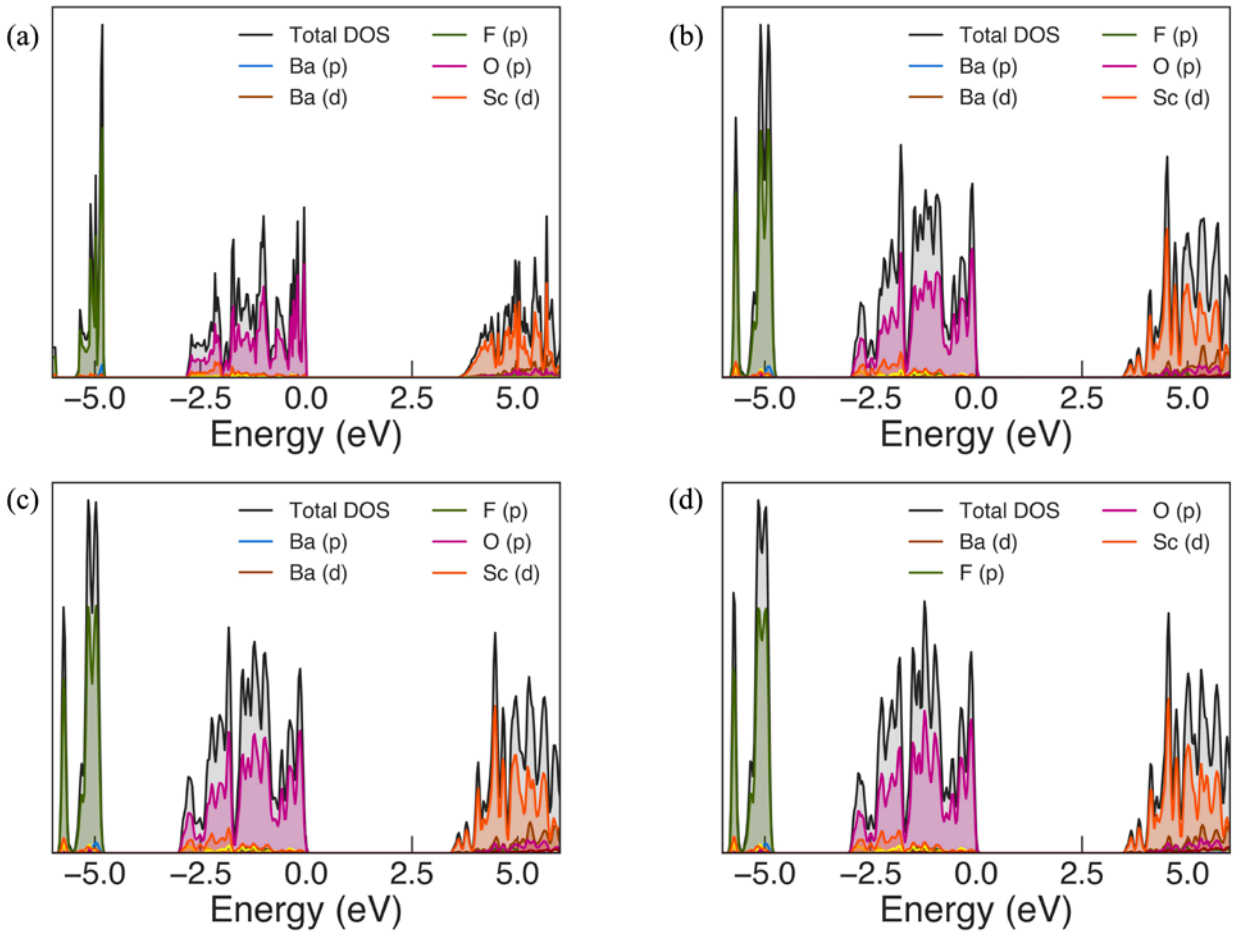


**Figure S3.** Electronic projected density of states for $Ba_{1-x}Sr_xScO_2F$ at $x$ = (a) 0 ($E_g$ = 3.58 eV) , (b) 0.09375 ($E_g$ = 3.57 eV), (c) 0.15625 ($E_g$ = 3.54 eV), and (d) 0.25 ($E_g$ = 3.60 eV). The conduction band minimum (CBM) is observed to have a high Sc-*d* orbital character.

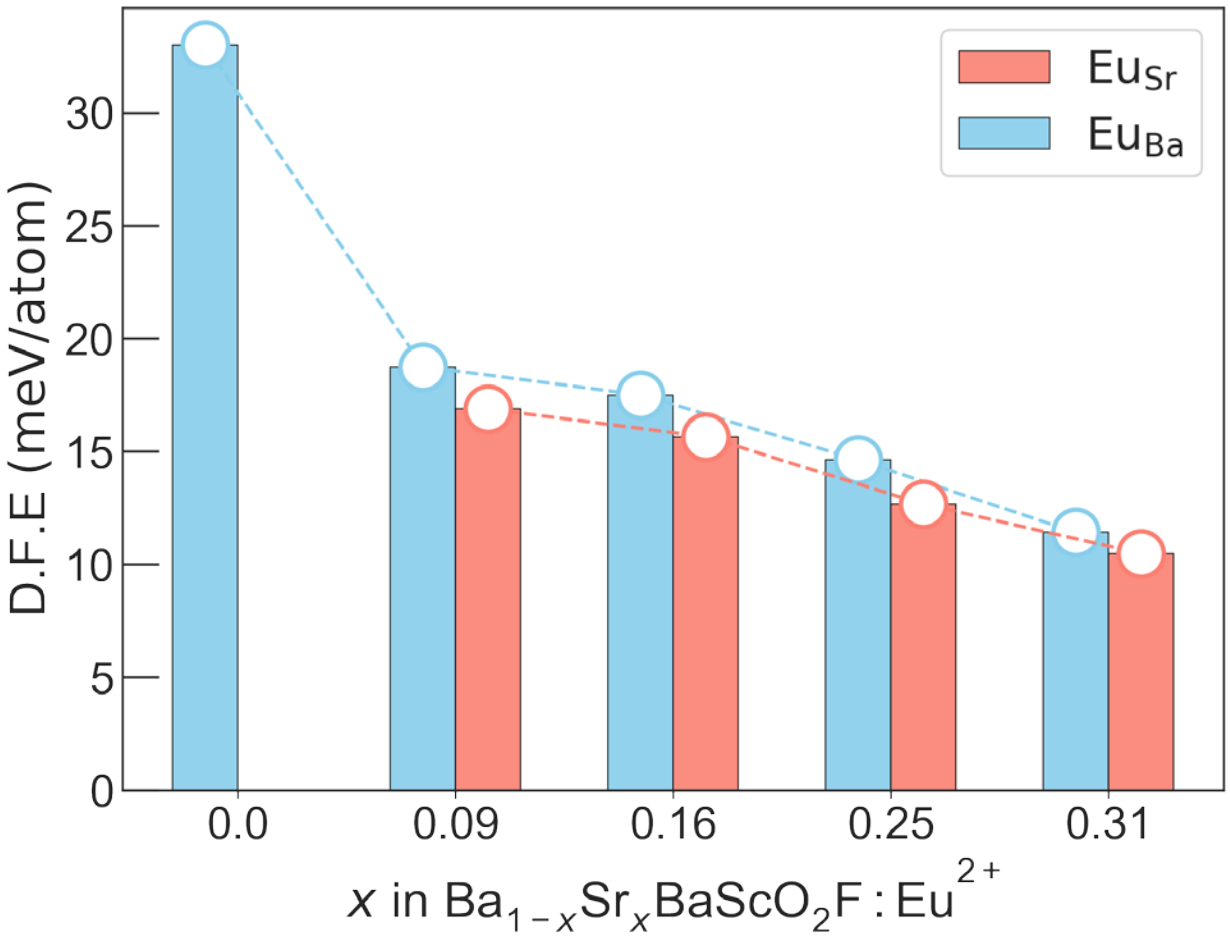


**Figure S4.** The dopant formation energy (D.F.E) of $Eu_{Sr}$ (red) and $Eu_{Ba}$ (blue) substitutions in $Ba_{1-x}Sr_xScO_2F$ ($x$ = 0, 0.09375, 0.15625, 0.25, 0.3125) expressed in meV per atom.

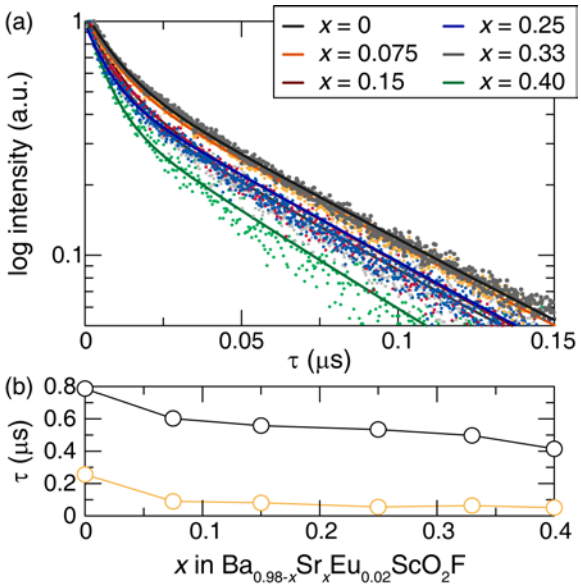


**Figure S5.** (a) Photoluminescent decay curves of $(Ba_{1-x}Sr_x)_{0.98}Eu_{0.02}ScO_2F$ ($x$ = 0.075, 0.15, 0.25, 0.33, 0.40) fit to a bi-exponential function and (b) the resulting lifetimes.

**Table S1.** Refined atomic positions, thermal parameters, and occupancies of $Ba_{0.566(2)}Sr_{0.433(8)}ScO_2F$

| Atom | Wyck. Pos. | $x$ | $y$ | $z$ | $U_{iso}$ (Å$^2$) | occ. |
|---|---|---|---|---|---|---|
| Ba | 1*b* | ½ | ½ | ½ | 0.0076(3) | 0.566(2) |
| Sr | 1*b* | ½ | ½ | ½ | 0.0076(2) | 0.433(8) |
| Sc | 1*a* | 0 | 0 | 0 | 0.0075(2) | 1 |
| O | 3*d* | ½ | 0 | 0 | 0.0250(9) | 0.667 |
| F | 3*d* | ½ | 0 | 0 | 0.0250(9) | 0.333 |

**Table S2.** Calculated lattice parameters and phase stability ($E_{hull}$) of $BaScO_2F$ for two lowest energy O/F configurations.

| **Phase** | ***P4$_2$/mmc*** | ***P4/mmm*** |
|---|---|---|
| **a (Å)** | 4.214 | 4.206 |
| **b (Å)** | 4.214 | 4.206 |
| **c (Å)** | 8.386 | 4.215 |
| ***α*(°)** | 90.0 | 90.0 |
| ***β*(°)** | 90.0 | 90.0 |
| ***γ*(°)** | 90.0 | 90.0 |
| ***E*$_{hull}$ (meV/atom)** | 93 | 98 |

**Table S3.** The computed $Eu^{2+}$ average bond length ($l_{avg}$) in Å.

| **$Ba_{1-x}Sr_xScO_2F:Eu^{2+}$** | **$l_{avg}$ (Å)** |
|---|---|
| ***x* = 0** | 2.78 |
| ***x* = 0.09375** | 2.71 |
| ***x* = 0.15625** | 2.66 |
| ***x* = 0.25** | 2.65 |
| ***x* = 0.3125** | 2.59 |