Electronic Supplementary Material (ESI) for RSC Advances

Luminescence of undoped and Eu^{3+} doped nanocrystalline $SrWO_4$ scheelite: Time resolved fluorescence complimented by DFT and Positron annihilation spectroscopic studies

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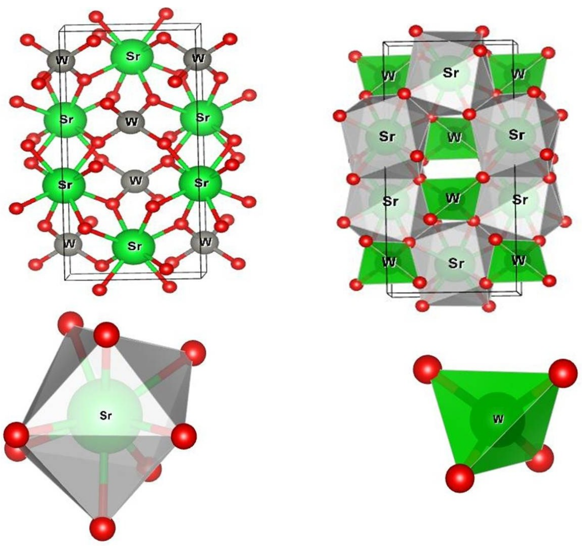

Figure S1: Crystal structure of Scheelite compound $SrWO_4$ along with SrO_8 and WO_4 polyhedra

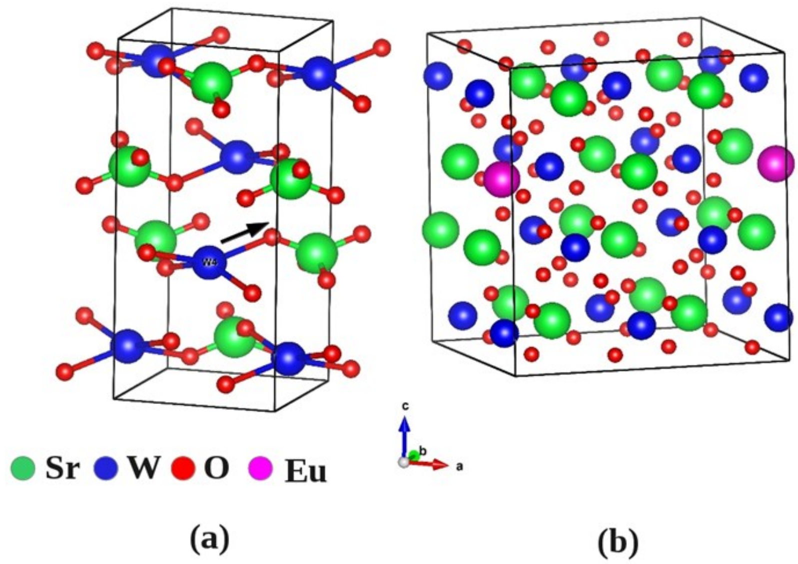

Figure S2: (a) Unit cell of $SrWO_4$ (24 atoms) and W atom situated at position (0.5, 0.25, 0.375) in direct lattice co-ordinate was displaced to generate distortion model (marked by arrow) (b) Eu doped 2x2x1 supercell (96 atoms) of $SrWO_4$, where one Eu ion was substituted in place of Sr.

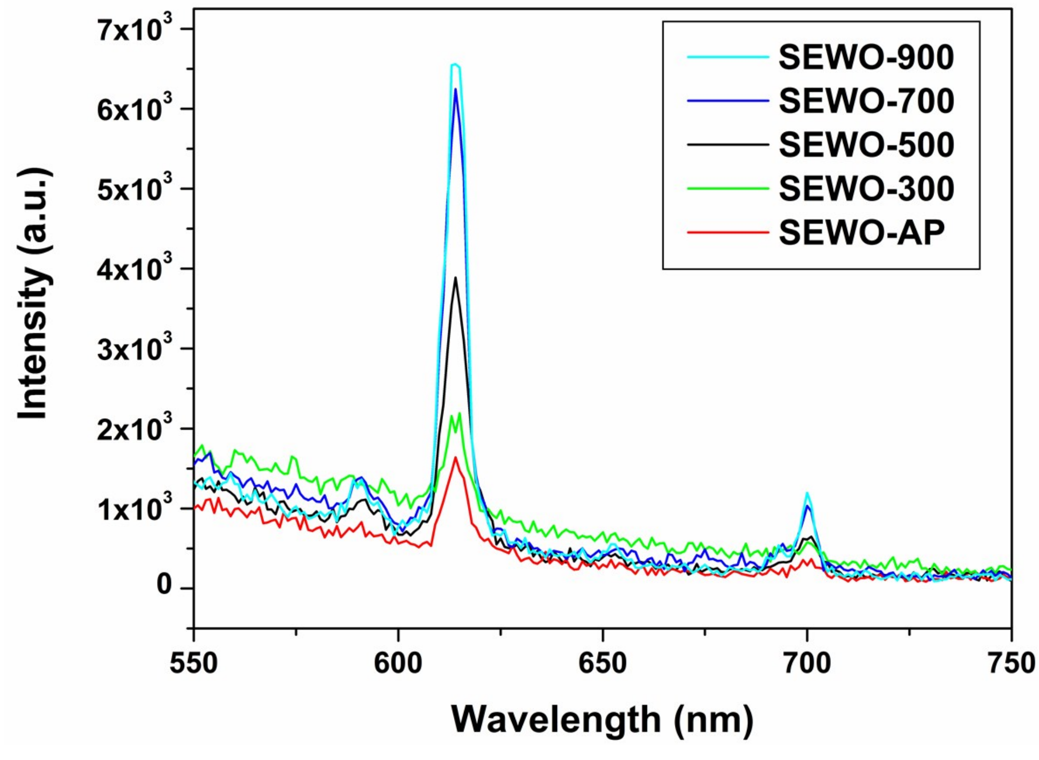

Figure S3: Emission spectra for Eu^{3+} doped $SrWO_4$ samples annealed at various temperature with λ_{ex}-395 nm.

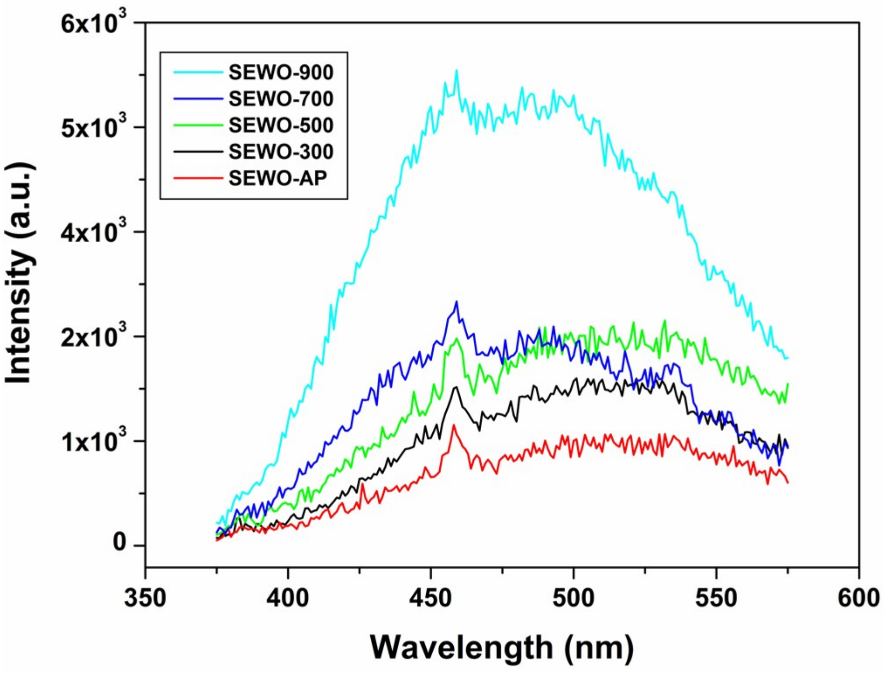

Figure S4: Host emission in the emission spectra of SEWO samples annealed at different temperatures

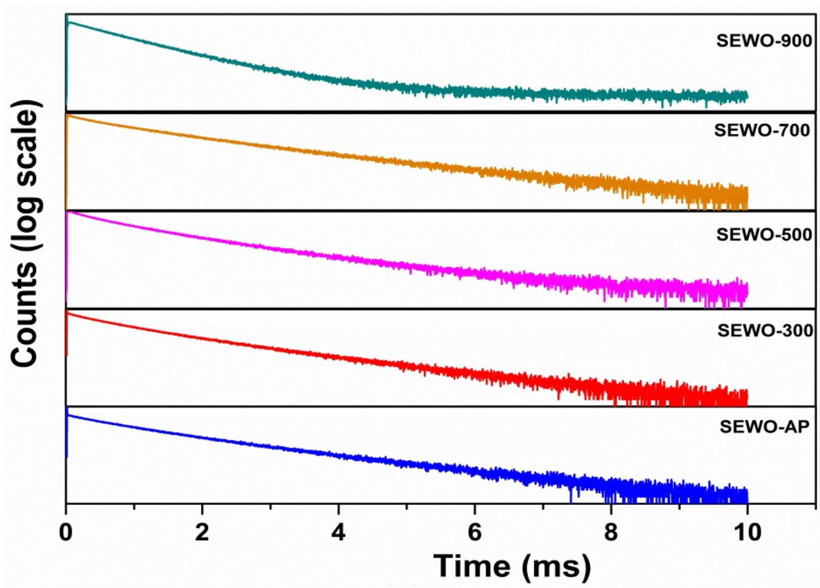

Figure S5: PL decay curve for the $^{5}D_{0}$ level of Eu^{3+} in $SrWO_4$: Eu samples annealed at different temperatures

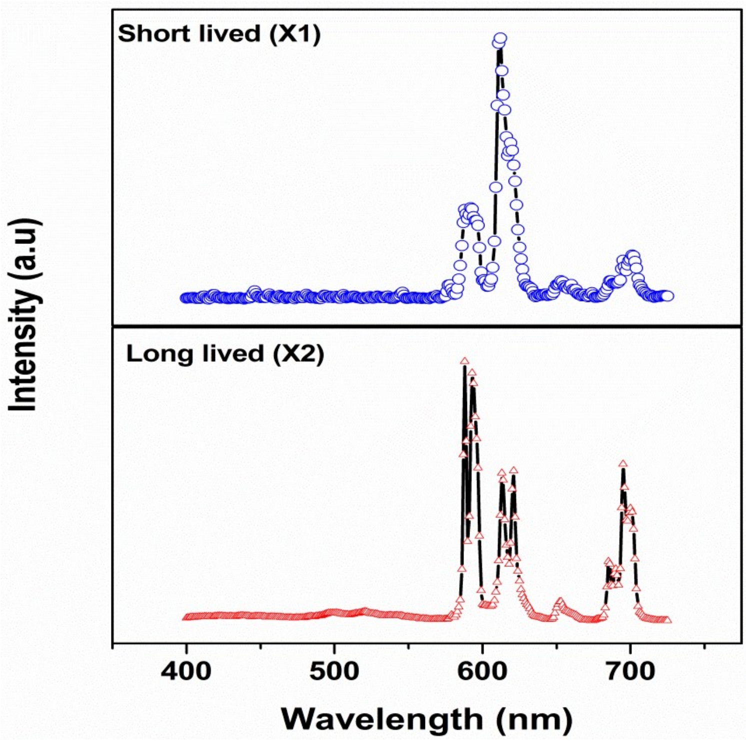

Figure S6: Time-resolved emission spectra of for short and long lived Eu^{3+} ion in SEWO-AP

Table T1: Comparison of PAW-PBE calculated and experimentally determined equilibrium lattice parameters, unit-cell volume, atomic positions, bond angles and electronic band gap of scheelite $SrWO_4$.

Property	Theory (this study)	Experiment [24]
Space Group	Tetragonal $I4_1/a$ (No. 88)	Tetragonal $I4_1/a$ (No. 88)
Lattice Parameters (Å) *a* *c*	 5.49488 12.13425	 5.421(5) 11.952(9)
Cell Volume (Å^3)	366.38	351.27(6)
Atomic positions Sr *4(b)* W *4(a)* O *16(f)*	 0.0 0.25 0.625 0.0 0.25 0.125 0.23699 0.11168 0.04290	 0.0 0.25 0.625 0.0 0.25 0.125 0.2683(2) 0.1093(2) 0.0496(7)
Bond lengths (Å) W-O Sr-O' Sr-O"	 1.80719 2.61093 2.65160	 1.873(3) 2.487(8) 2.552(3)

Bond angle Sr-O-Sr Sr-O-W Sr-O''-W O'-W-O' O''-W-O''	 102.1023 120.0555 134.9582 107.6918 113.0918	 106.37 (3) 122.36 (3) 130.82 (4) 103.38 (7) 122.49 (6)
Band-gap (eV)	4.00	4.60 [24], 5.06 [50]

Table T2: CIE color coordinate of $SrWO_4$ crystallite obtained at different temperature

Sample	**Symbol in CIE diagram**	**(x, y)**
SWO-AP	A	(0.30, 0.36)
SWO-300	B	(0.29, 0.35)
SWO-500	C	(0.33, 0.37)
SWO-700	D	(0.24, 0.29)
SWO-900	E	(0.26, 0.31)

Table T3: Procedure data slicing in TRES

- **Supposing there are two components A (short lived) and B (long lived), first we record the composite spectrum (A+B) with very short delay (just to avoid the lamp profile).**
- **Then give sufficient delay and record with identical integration times so that there is only B component in the spectrum (let's say B'; A is already decayed).**
- **But the intensity of the B' which we would get is not the same as the original B in the composite spectrum (A+B).**
- **So we multiply a suitable multiplying factor (exp factor, $e^{-t/\tau}$) so as to get the original intensity of B.**
- **Then if we subtract this B from the composite spectrum (A+B), it is possible to get the short lived component A.**

One has to maintain however same gate widths while dealing with this type of procedure