

†Electronic Supplementary Information (ESI)

Bane to boon: Tailored defect induced bright red luminescence from Cuprous Iodide nanophosphors for *on-demand* rare earth free energy saving lighting applications

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Figure S1: Digital images of the precipitated CuI in the solution (a) just before putting into the autoclave and (b) after the hydrothermal reaction. Long time of hydrothermal reaction makes the solution transparent indicating the entrapment of the excess iodine into the already precipitated CuI.

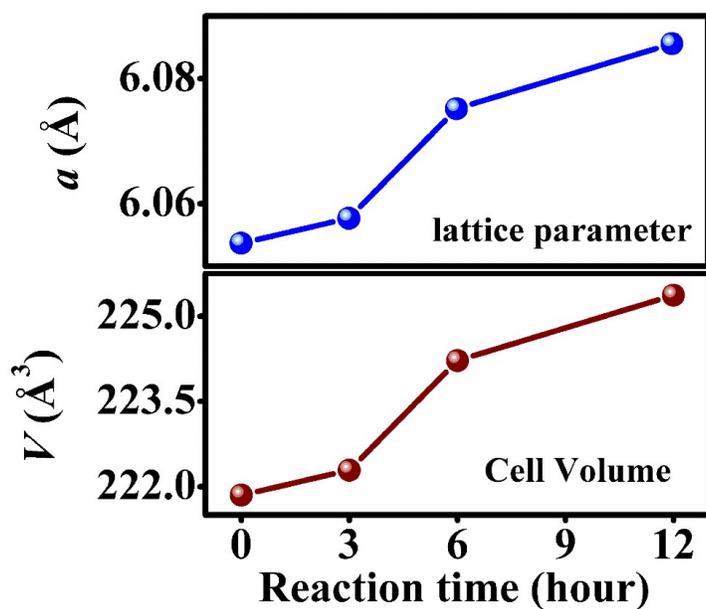


Figure S2: Variation of lattice parameter and cell volume with the hydrothermal reaction time

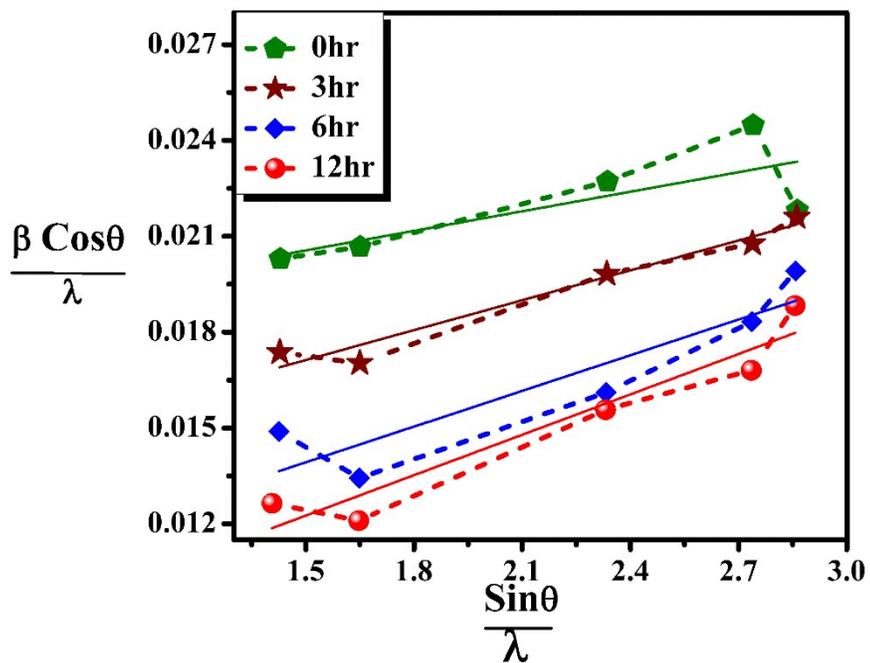


Figure S3: Williamson-Hall plot of the nanocrystals representing enhanced lattice strain with hydrothermal reaction time.

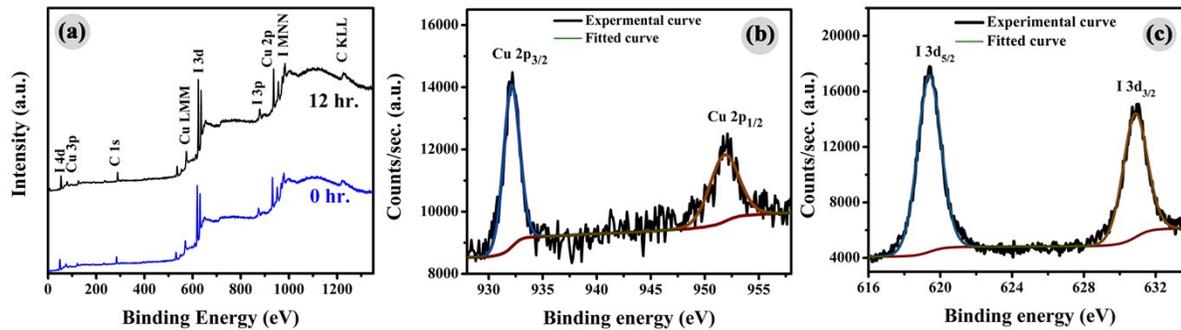


Figure S4: (a) Survey scan of the CuI nanophosphors evidently shows the full indexing of all the peaks which strongly discards any possibility of having impurity species. (b&c) Fitting of Cu 2p and I 3d core level high resolution scan representing the existence of only one valence state of the corresponding elements in the sample.

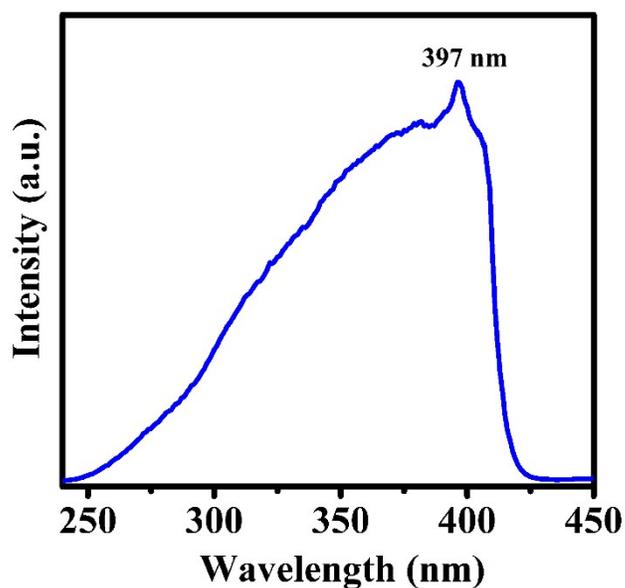


Figure S5: Photoluminescence excitation spectra of the CuI nanocrystals monitored at 688 nm

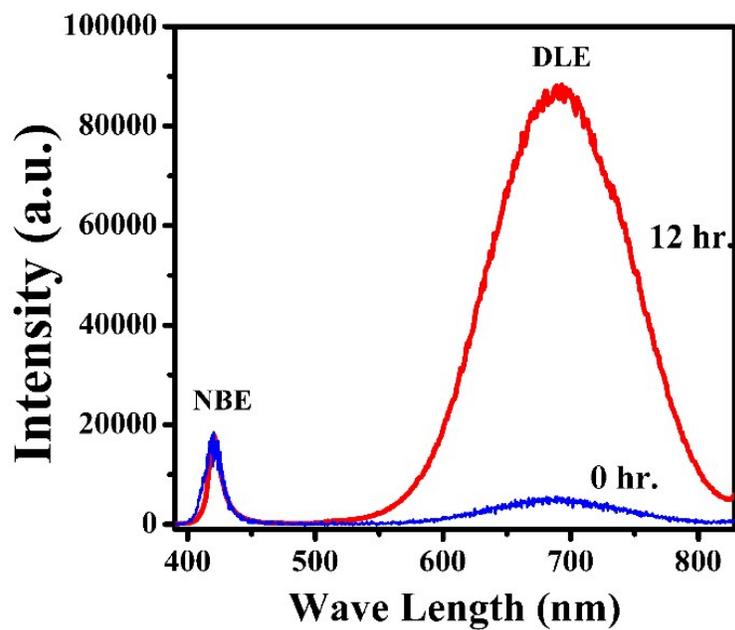


Figure S6: The cathodoluminescence spectra of the CuI nanocrystals under low voltage electron beam excitation (5 kV) for different reaction times. Both the samples show exactly the same nature as obtained from PL spectra.

Decay characteristics measurement:

The decay curves of 421 nm and 688 nm emission for CuI nanophosphors were well fitted into bi-exponential function. The double exponential decay function can be described by the following equation-

$$I(t) = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right)$$

Where τ_1 and τ_2 are the decay lifetimes of the luminescence, and A_1 and A_2 are the weighting parameters. The average lifetime for bi-exponential decay can be described by the equation -

$$\tau_{avg} = \frac{A_1 \tau_1^2 + A_2 \tau_2^2}{A_1 \tau_1 + A_2 \tau_2}$$

All the decay parameters are listed in the table below-

| Emission wavelength | A₁ | τ₁(ns) | A₂ | τ₂(ns) | τ_{avg} |
|----------------------------|----------------------|--------------------------|----------------------|--------------------------|------------------------|
| 421 nm | 0.8146 | 0.12411 | 0.1854 | 1.7572 | 1.37 ns |
| 688 nm | 0.3947 | 949.2051 | 0.6053 | 2853.4132 | 2.82 μs |

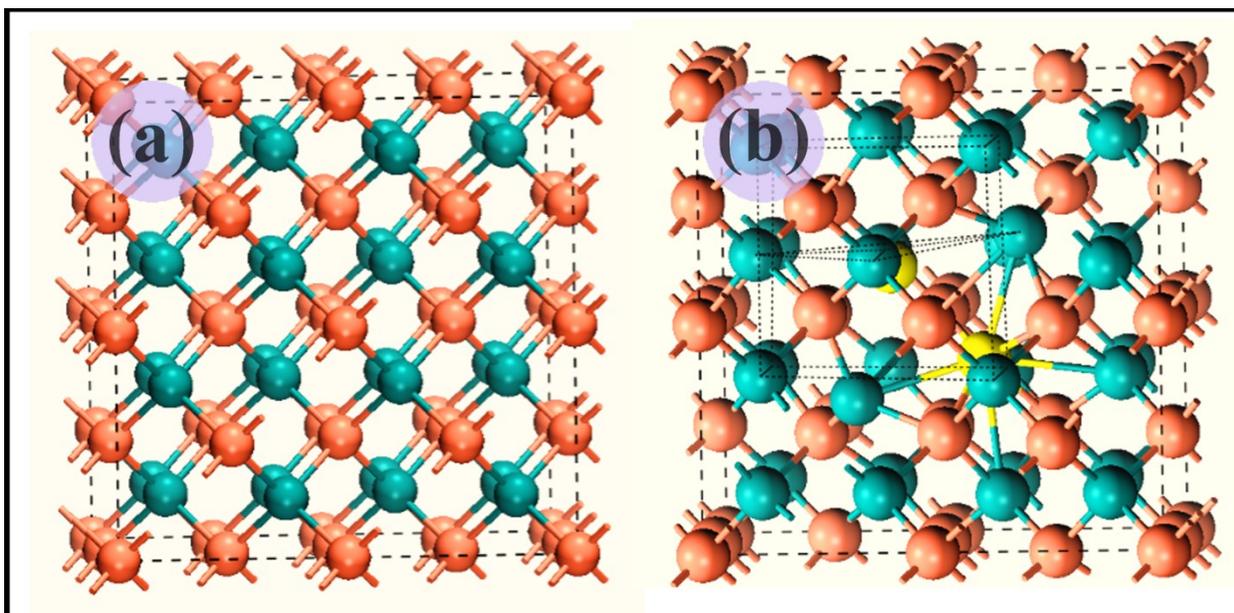


Figure S7: Demonstration of two $2 \times 2 \times 2$ supercell structures containing 32 Cu atoms and 32 I atoms for the pure CuI (a) while to investigate the effect of interstitial I , two I atoms were introduced (as indicated by the yellow atoms) in the two octahedral void position of the optimized pure structure (b).

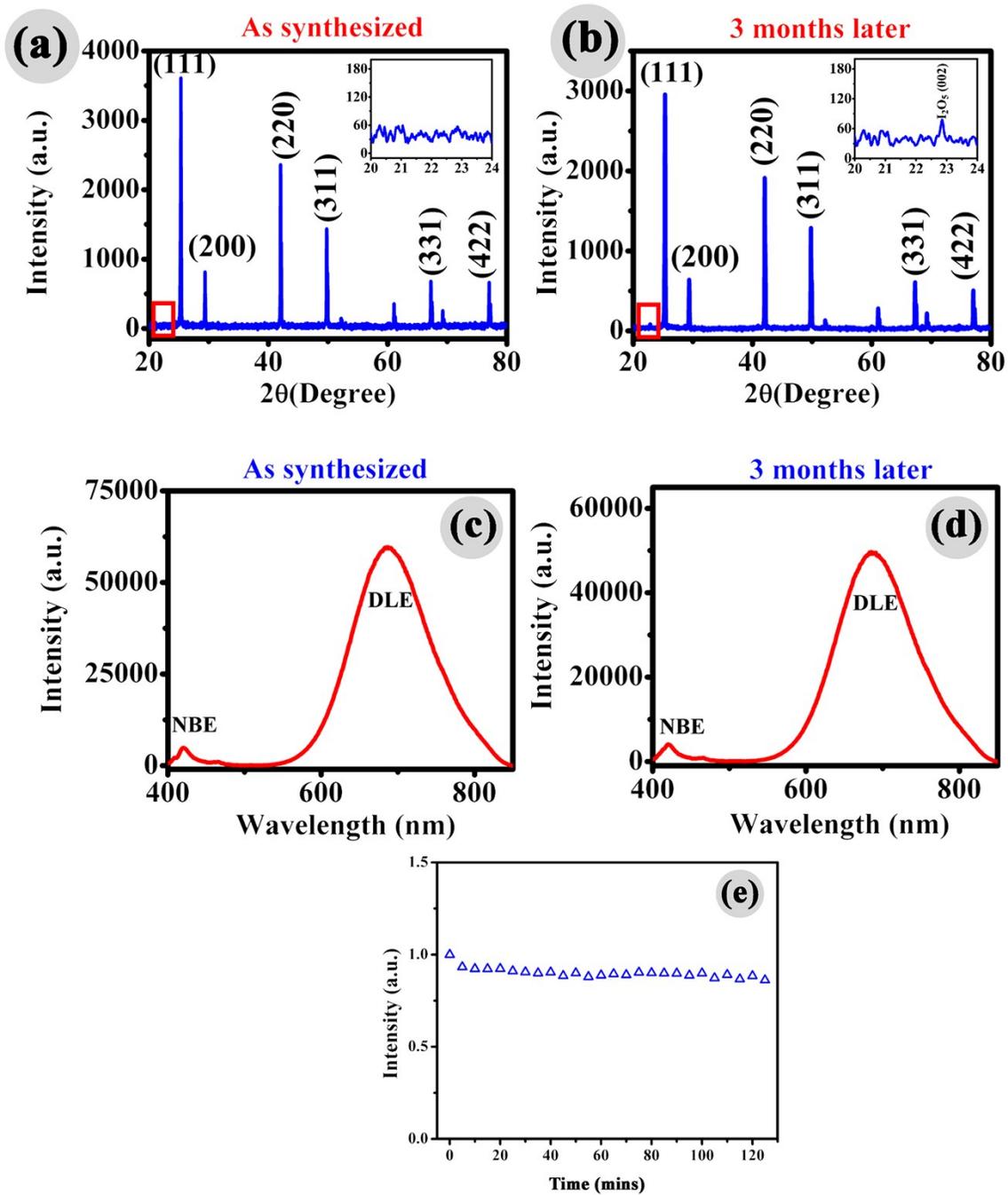


Figure S8: (a&b) and (c&d) Stability of the CuI nanophosphors is demonstrated by their respective XRD and PL pattern taken for as synthesized samples and after 3 months. Inset shows the selected magnified region to indicate the appearance of the peak corresponding to (002) plane

of I_2O_5 as indexed in JCPDS card no. 220338 (e) Demonstration of EL stability of CuI nanophosphor.