Scintillation Kinetics through DFT

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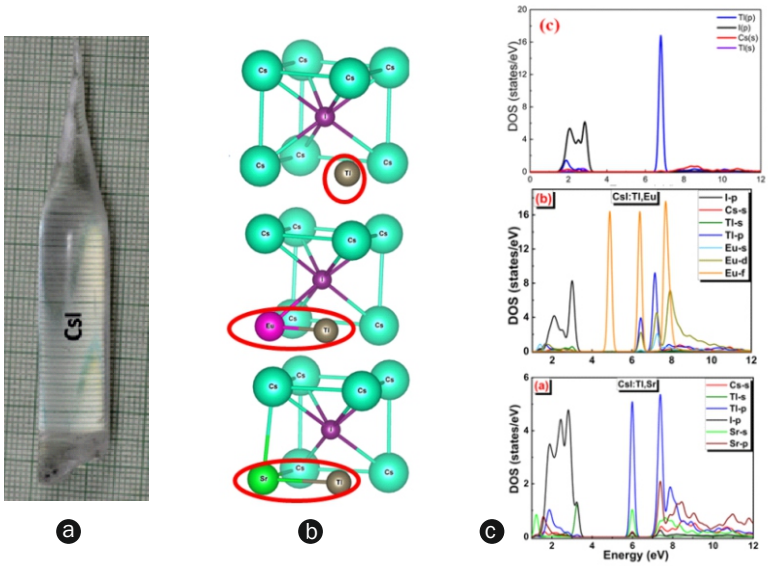
Electronic Structure Analysis to Understand Scintillation Kinetics of CsI Scintillator Single Crystal



(a) A CsI single crystal developed in BARC.
(b) Local crystal structure of CsI:Tl, CsI:Tl, Eu and CsI:Tl, Sr.
(c) Calculated partial density of states (PDOS) of CsI:Tl (Top) and defect complex and $Tl^{-}_{Cs}+Eu^{+}_{Cs}$ (middle) and $Tl^{-}_{Cs}+Sr^{+}_{Cs}$ (bottom) in CsI matrix.

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Among the conventional scintillators, CsI:Tl is widely used for gamma spectrometry. Other than having a very high light yield, CsI:Tl has an important ability of differentiating between the incoming radiation based on pulse shape discrimination (PSD). This differentiation arises from the presence of "short" and "long" decay component in the scintillation pulse. Divalent cation co-doping in CsI:Tl are one of the ways of tailoring the electronic structure so as to increase its PSD ability and simultaneously reducing the afterglow.

In a recent study (Sisodiya et al, Optimizing the Scintillation Kinetics of CsI Scintillator Single Crystal by Divalent Cation Doping: Insights from Electronic Structure Analysis and Luminescence Studies, J. Phys. Chem. C, doi.org/10.1021/acs.jpcc.3c06098), experimental investigations along with electronic structure calculations were carried out to understand scintillation kinetics of pure CsI, and doped/co-doped with Tl, Sr and Eu. DFT based electronic structure calculations showed that DX like defect center are formed in the CsI:Tl matrix when co-doped with Sr^{2+} and Eu^{2+} which effects its scintillation kinetics. The study gave an understanding of how the defects need to be tailored to enhance the properties of CsI:Tl.