Researchers unveil local electronic structure of lanthanide-doped double perovskites
26 October 2022, by Liu Jia

Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences introduced Yb$^{3+}$ into Cs$_2$NaInCl$_6$ DPs and realized efficient NIR luminescence with the optimal photoluminescence quantum yields (PLQY) of 39.4%.

The researchers unveiled the local electronic structure of Cs$_2$NaInCl$_6$:Yb$^{3+}$ through density functional theory calculation and Bader charge analysis, which indicated that electrons in [YbCl$_6$]$^{3-}$ octahedron were strongly localized in Cs$_2$NaInCl$_6$:Yb$^{3+}$, while they were delocalized toward Ag$^+$ in Cs$_2$AgInCl$_6$:Yb$^{3+}$. Such a localized electron can effectively boost the NIR luminescence via Cl$^-$-Yb$^{3+}$ charge transfer sensitization in Cs$_2$NaInCl$_6$.

Benefiting from the localized electrons of [YbCl$_6$]$^{3-}$ octahedron in Cs$_2$NaInCl$_6$ DPs, an efficient strategy of Cl$^-$-Yb$^{3+}$ charge transfer sensitization was proposed to obtain intense NIR luminescence of Ln$^{3+}$.

The researchers demonstrated the proposed novel sensitization strategy for enhancing the NIR emission of Ln$^{3+}$ to be superior to the self-trapped excitons sensitization in the well-established Cs$_2$AgInCl$_6$ counterparts.

They carried out temperature-dependent steady-state and transient PL spectroscopic measurements to verify the Cl$^-$-Yb$^{3+}$ charge transfer process in Cs$_2$NaInCl$_6$:Yb$^{3+}$ by the characteristic transition from charge transfer band (CTB) to $^{2}F_{7/2}$ (Yb$^{3+}$) and $^{2}F_{5/2}$ (Yb$^{3+}$).

Density functional theory calculation and Bader charge analysis indicated that the [YbCl$_6$]$^{3-}$ octahedron is strongly localized in Cs$_2$NaInCl$_6$:Yb$^{3+}$, which facilitates the Cl$^-$-Yb$^{3+}$ charge transfer.
Furthermore, the researchers achieved efficient NIR luminescence from Er\(^{3+}\) with PLQY of 7.9% in Yb\(^{3+}/Er^{3+}\) co-doped Cs\(_2\)NaInCl\(_6\) DPs due to the energy transfer from Cl\(^-\)-Yb\(^{3+}\) CTB to Er\(^{3+}\).

These findings provide a general approach to achieve effective NIR emission of Ln\(^{3+}\) in halide DPs, opening up a new avenue for exploring NIR-emitting perovskite derivatives toward versatile applications.


Provided by Chinese Academy of Sciences

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