Supporting Information

Highly efficient yellow emission and abnormal thermal quenching in Mn^{2+} doped Rb_4CdCl_6

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Computational details

All the calculations are performed in the framework of the density functional theory with the projector augmented plane-wave method, as implemented in the Vienna ab initio simulation package[1]. The generalzied gradient approximation proposed by Perdew, Burke, and Ernzerhof is selected for the exchange-correlation potential[2]. The cut-off energy for plane wave is set to 500 eV. The energy criterion is set to 10^{-6} eV in iterative solution of the Kohn-Sham equation. The unit cell of Rb_4CdCl_6 and Rb_4CdCl_6:Mn^{2+} is relaxed until the residual forces on the atoms have declined to less than 0.01 eV/Å. The Brillouin zone integration is performed using dense $6 \times 12 \times 4$ Monkhorst-Pack grids for electronic structure calculation. The band structure is calculated with hybrid PBE0 functional.

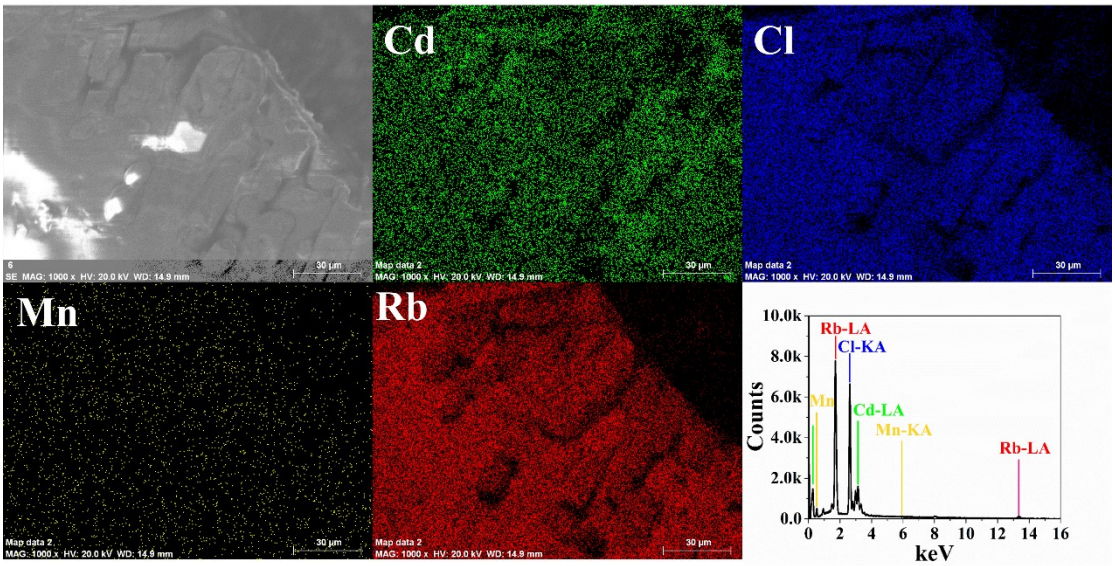

Figure S1. (a) SEM mapping of $Rb_4CdCl_6:Mn^{2+}$. (b-f) Corresponding elemental mapping analysis for Cd, Cl, Mn and Rb.

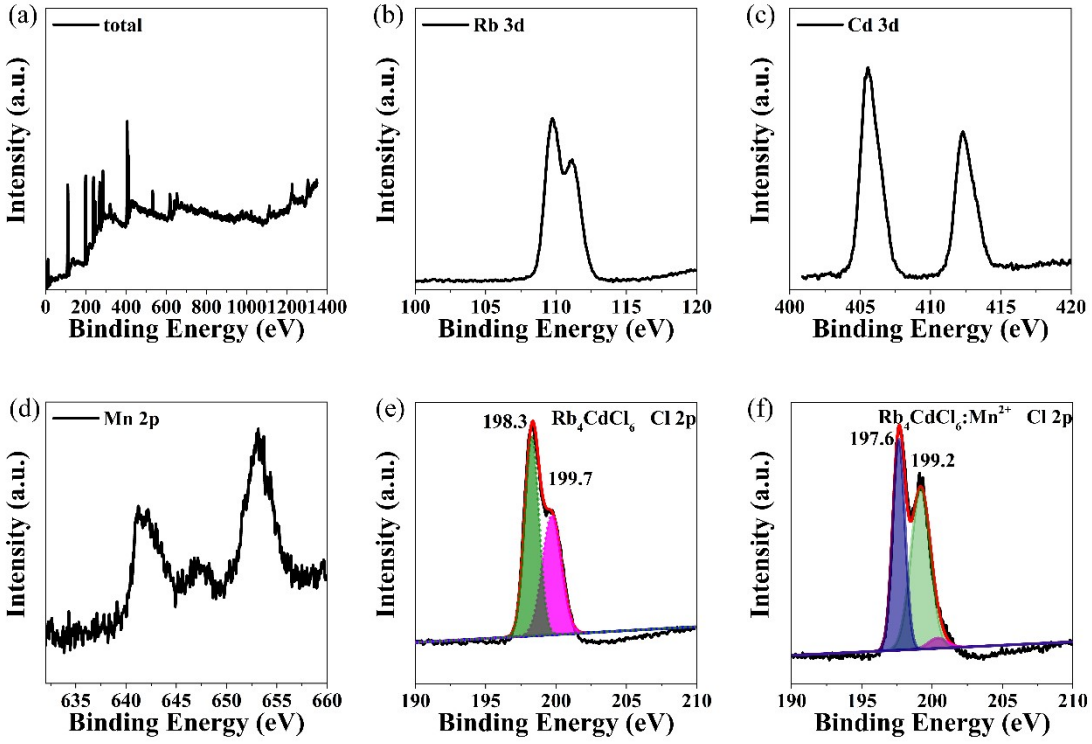

Figure S2. (a-e) XPS spectra corresponding to Rb_4CdCl_6, Rb, Cd, Mn and Cl. (f) XPS spectrum of Cl in Rb_4CdCl_6:Mn^{2+}.

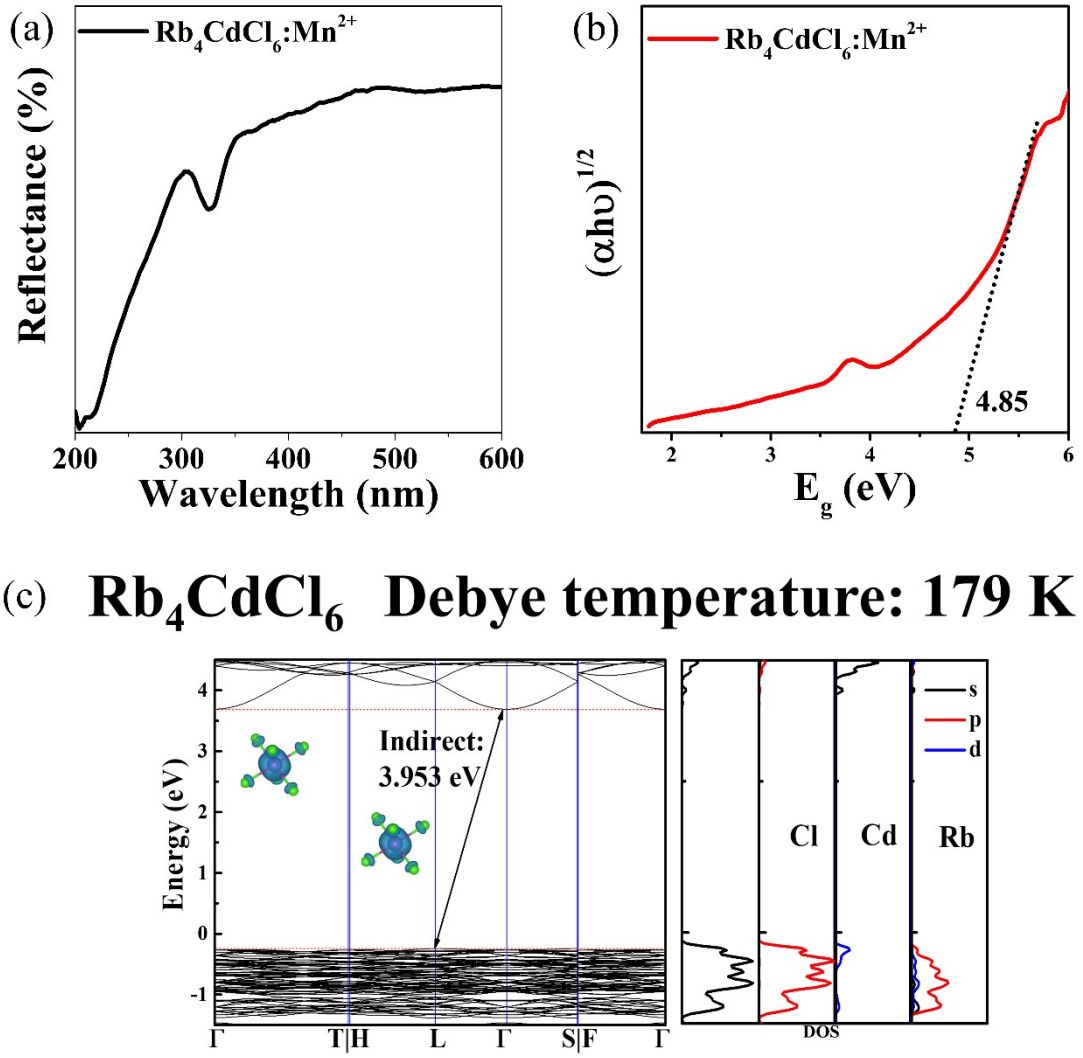

Figure S3. (a) UV-vis reflection spectra for $Rb_4CdCl_6:Mn^{2+}$. (b) Relationship of $[\alpha hv]^{1/2}$ and photon energy hv showing indirect band gaps for $Rb_4CdCl_6:Mn^{2+}$. (c) Debye temperature and calculated electronic structure for Rb_4CdCl_6.

Reference

1. Kresse, G.; Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **1999,** 59 (3), 1758-1775.

2. Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996,** 77 (18), 3865-3868.