

## **Supporting information**

FIG S1. Geometric structures of  $Cs_2AgInCl_6$  supercells containing  $Mn_{CS}$  defect. The red circles represent Mn atom. The green, purple, blue and brown atoms represent Cl, Cs, Ag and In atoms, respectively.



FIG S2. Geometric structures of  $Cs_2AgInCl_6$  supercells containing  $Mn_{In}$  defect, Numbers in all figures represent the bond lengths and bond angles, respectively. The red circles represent Mn atom. The green, purple, blue and brown atoms represent Cl, Cs, Ag and In atoms, respectively.



FIG S3. Geometric structures of  $Cs_2AgInCl_6$  supercells containing  $Mn_{Ag}V_{Cs}$  defect, Numbers in all figures represent the bond lengths and bond angles, respectively. The red circles represent Mn atom. The green, purple, blue and brown atoms represent Cl, Cs, Ag and In atoms, respectively.



FIG S4. Geometric structures of  $Cs_2AgInCl_6$  supercells containing  $Mn_{Ag}Mn_{In}$  defect, Numbers in all figures represent the bond lengths and bond angles, respectively. The red circles represent Mn atom. The green, purple, blue and brown atoms represent Cl, Cs, Ag and In atoms, respectively.