Supporting Information for

Investigation of Fe^{2+} incorporated organic-inorganic hybrid perovskites from first principles and experiments

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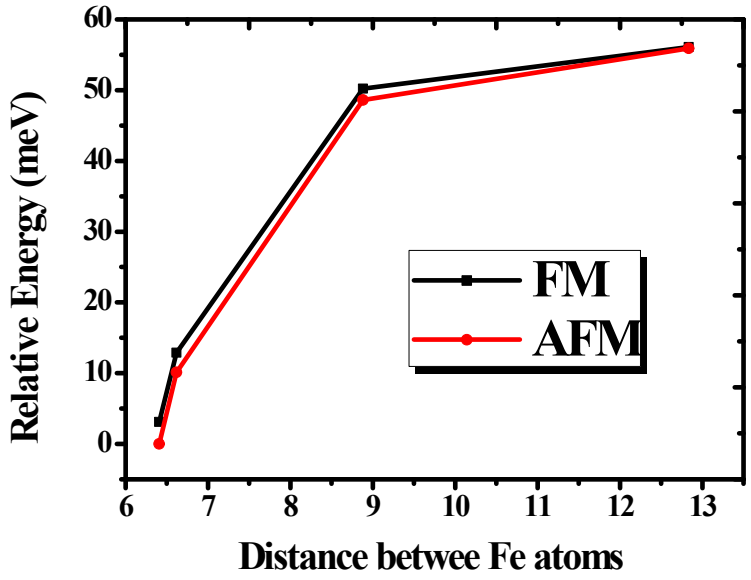


Figure S1. Relative energies of four different configurations as the pair distance changes for both AFM and FM phases. The total energy of configuration I under AFM state is set to zero as a reference.

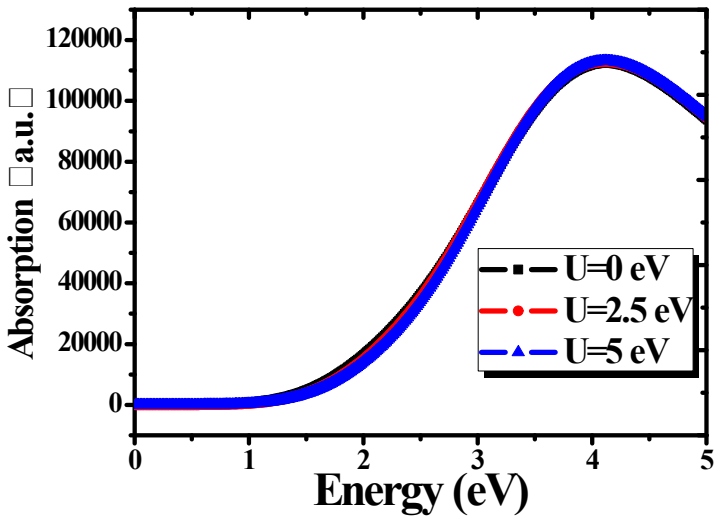


Figure S2. Intensity of the absorption with DFT+*U* (*U*=0, 2.5, 5 eV).

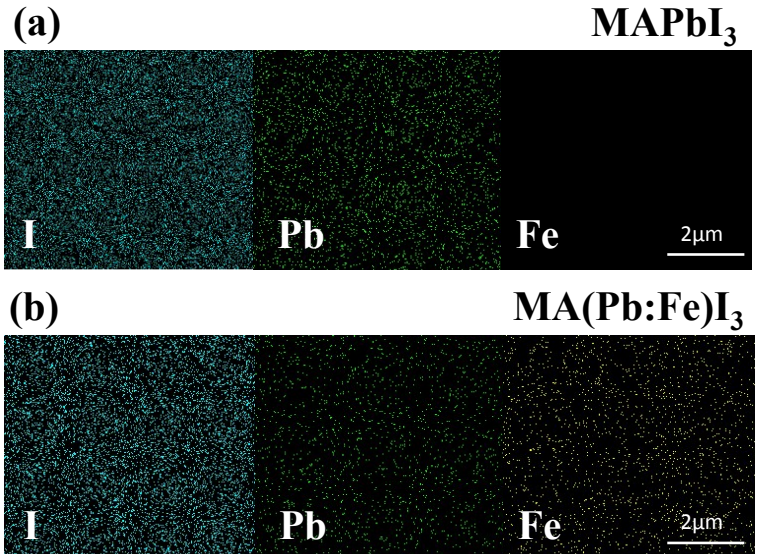


Figure S3. EDX elemental mapping of (a) $MAPbI_3$ and (b) $MA(Pb:Fe)I_3$.

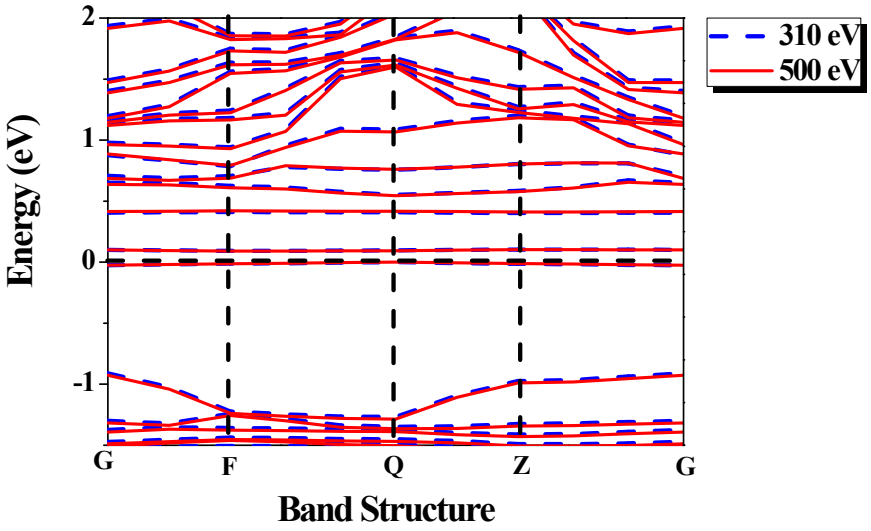
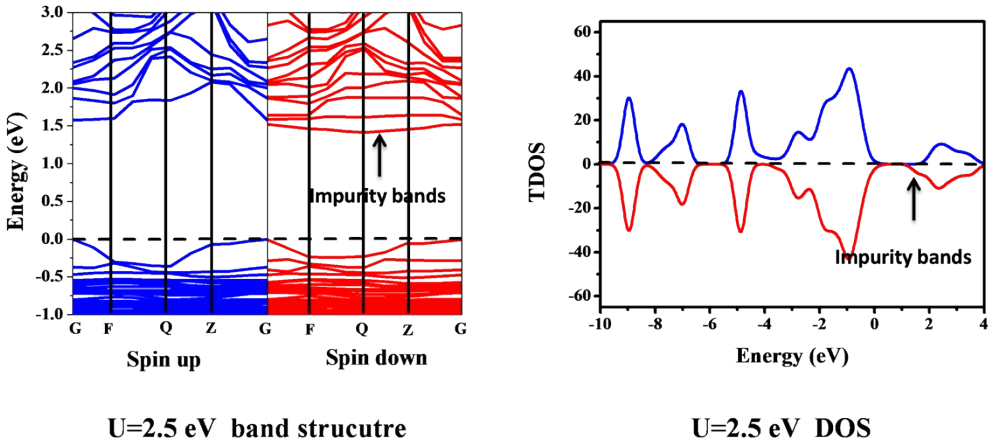
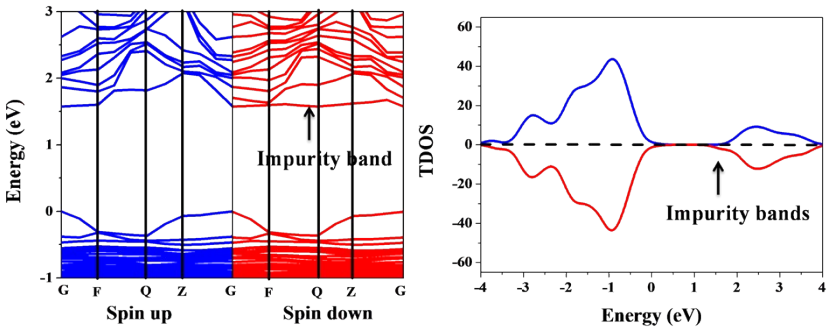


Figure S4. Band structure based on the cutoff with 310 eV and 500 eV with 12.5 at.% Fe doped perovskite.



U=2.5 eV band strucutre **U=2.5 eV DOS**

Figure S5. Band structure and DOS of the 12.5 at.% Fe doped perovskite with DFT+U (U=2.5 eV).



U=5 eV Band strucutre **U=5 eV DOS**

Figure S6. Band structure and DOS of the 12.5 at.% Fe doped perovskite with DFT+U (U=5 eV).