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# Electronic Structure of Organic-Inorganic Lanthanide Iodide Perovskite Solar Cell Materials

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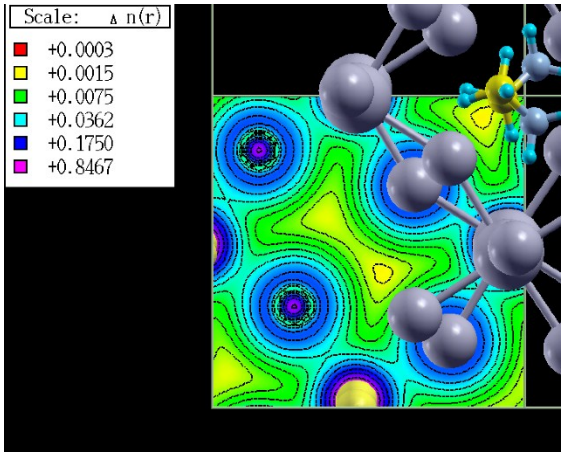
## Supporting Information

Table S1,S2- lattice constant (a,b,c tetragonal) of the lanthanide perovskite materials in Cartesian units and the normalized geometrical factors versus leas iodide perovskite(U=5).

| Compound | $\frac{a(La)}{a(Pb)}$ | $\frac{b(La)}{b(Pb)}$ | $\frac{c(La)}{c(Pb)}$ | $\frac{a_H(La)}{a_H(Pb)}$ | $\frac{a_V(La)}{a_V(Pb)}$ | $\alpha_H(La)-\alpha_H(Pb)[^\circ]$ | $\alpha_V(La)-\alpha_V(Pb)[^\circ]$ | $\Theta(La)-\Theta(Pb)[^\circ]$ |
|---|---|---|---|---|---|---|---|---|
| $MAEuI_3$ | 1.003 | 1.003 | 1.005 | 1.004 | 1.005 | 2.6 | 0.43 | 0.69 |
| $MADyI_3$ | 0.98 | 0.98 | 0.97 | 0.98 | 0.96 | 3.7 | 0.55 | -1.1 |
| $MATmI_3$ | 0.98 | 0.97 | 0.99 | 0.99 | 0.98 | 0.71 | 0.83 | 4.8 |
| $MAYbI_3$ | 0.97 | 0.96 | 0.95 | 0.96 | 0.94 | 4.1 | 2.2 | -3.6 |

| Compound | a [Å] | b [Å] | c [Å ] | c/a | $a_H$ [Å] | $a_V$ [Å] | $\alpha_H$ [°] | $\alpha_V$ [°] | $\Theta$ [°] |
|---|---|---|---|---|---|---|---|---|---|
| $MAEuI_3$ | 8.92 | 8.98 | 13.28 | 1.48 | 3.26 | 3.33 | 175.5 | 172.6 | 27.2 |
| $MADyI_3$ | 8.73 | 8.75 | 12.79 | 1.46 | 3.17 | 3.21 | 176.6 | 172.7 | 25.4 |
| $MATmI_3$ | 8.72 | 8.72 | 13.04 | 1.50 | 3.21 | 3.27 | 173.6 | 173.0 | 31.3 |
| $MAYbI_3$ | 8.60 | 8.63 | 12.53 | 1.46 | 3.11 | 3.14 | 177.0 | 174.4 | 22.9 |




FigS1- Charge density profile of MAPbI3

**Fig. S2-** Optimized atomic configuration within the perovskite unit cell for lanthanide iodide perovskite materials. The considered lantanide elements are Eu(a), Dy(b), Tm(c) and Yb(d).

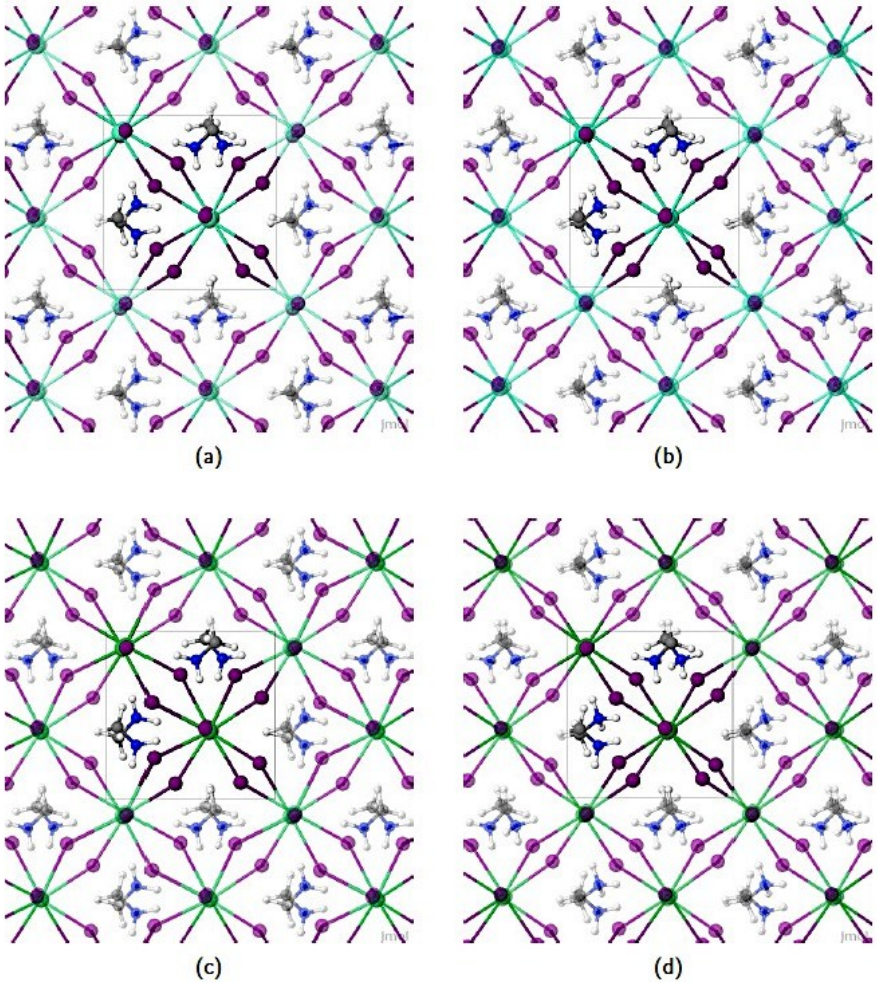


Fig.S3- Data for Electronic structure and charge density of lanthanide iodide perovaskites from GGA+U calculations(U=5).

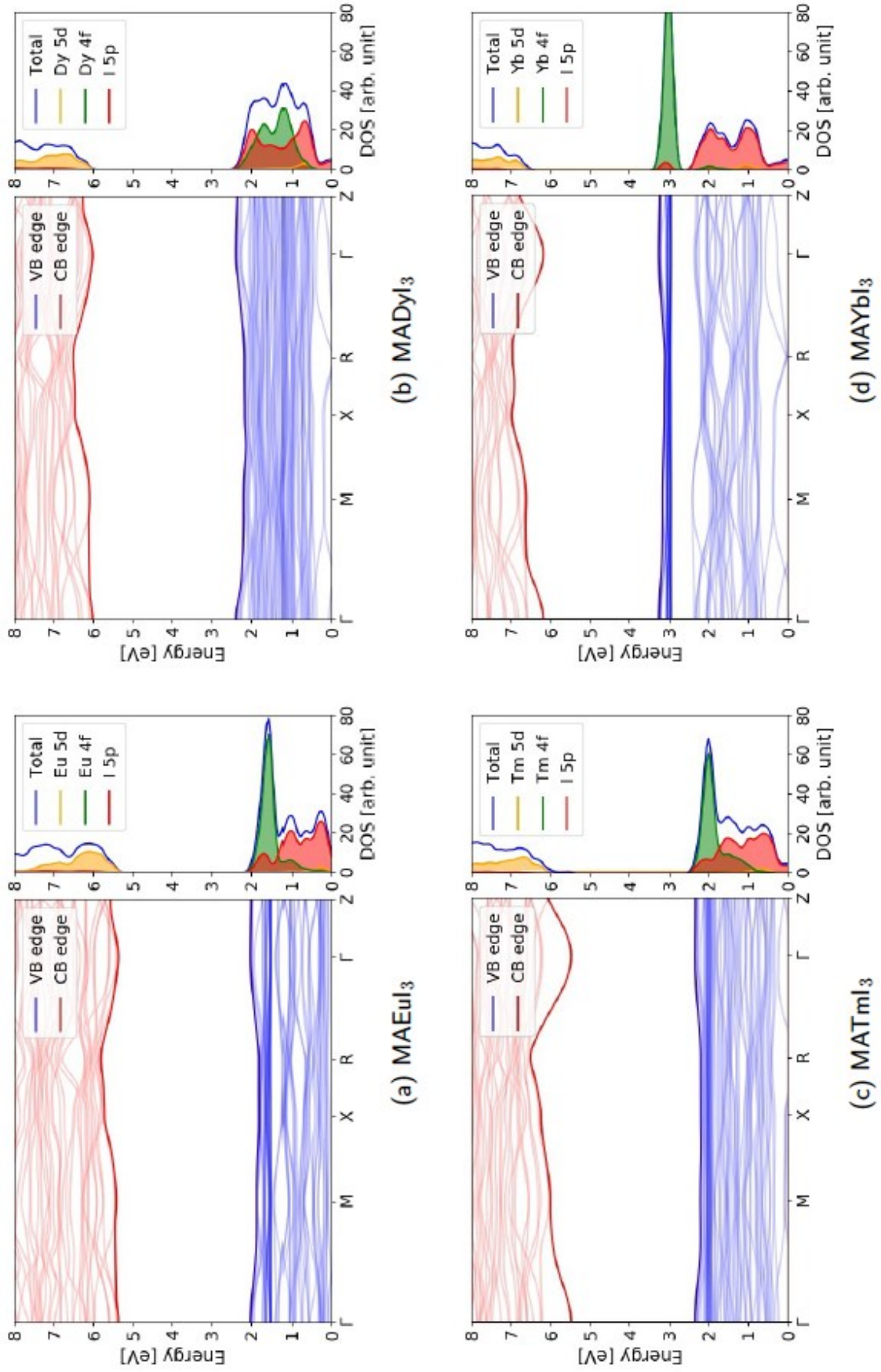


Fig.S4 Charge density plots of the lanthanide perovskites calculated by U=5.

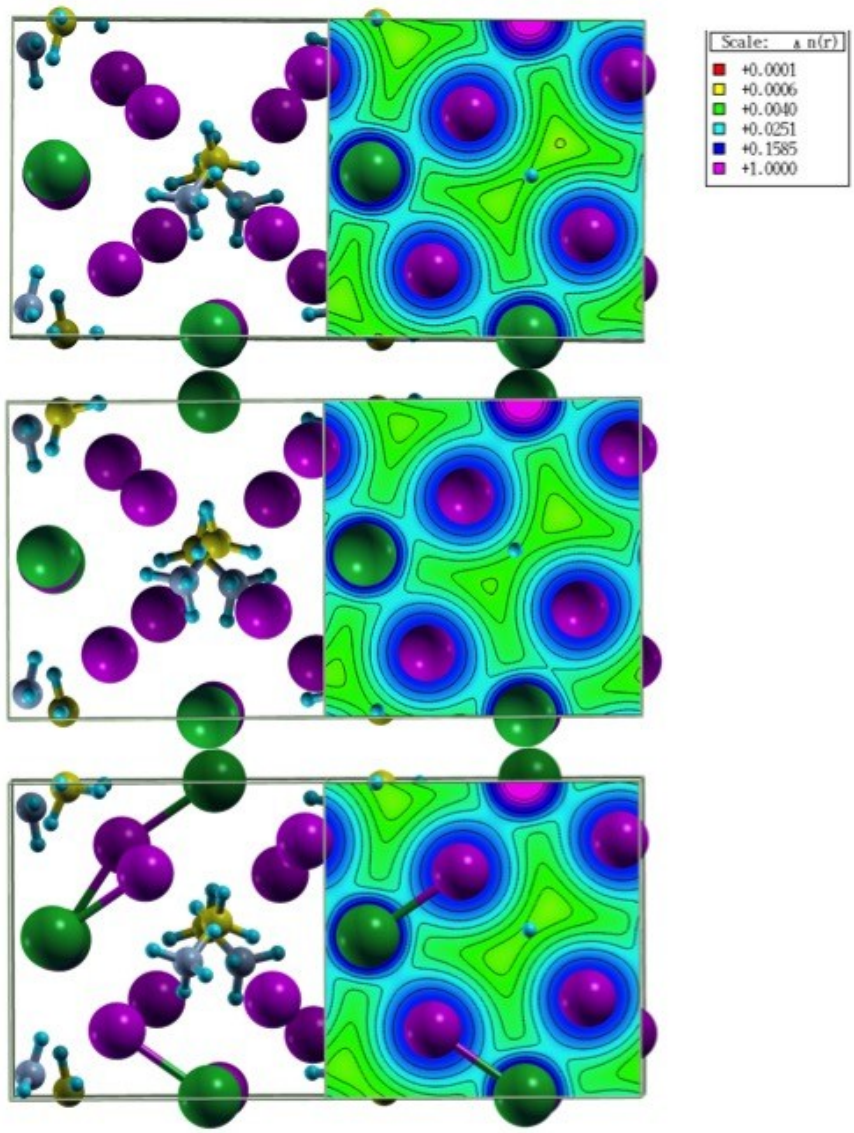



Table S3- Geometrical factors for lanthanide iodide perovskites from optimized coordinates calculated by Hubbard U=3.

| | a (Å) | b (Å) | c (Å) | $\alpha_H$(°) | $\alpha_V$(°) | $a_H$(Å) | $a_V$(Å) |
|---|---|---|---|---|---|---|---|
| **$MAEuI_3$** | 8.92 | 8.98 | 13.28 | 3.25 | 3.33 | 176.7 | 175.02 |
| **$MATmI_3$** | 8.80 | 8.82 | 12.89 | 3.16 | 3.23 | 177.5 | 174.87 |
| **$MAYbI_3$** | 8.71 | 8.74 | 12.69 | 3.14 | 3.17 | 176.72 | 172.2 |

Table S4- Effective mass of charge carriers for investigated lanthaniode iodide perovskite materials defined in the units of free electron mass(m0). f in valence pseudopotentials together with Hubbard u=5 were implemented.

| Direction | Γ-M $m_e^*/ m_h^*$ [m0] | Γ-R $m_e^*/ m_h^*$ [m0] | Γ-Z $m_e^*/ m_h^*$ [m0] | Average $m_e^*/ m_h^*$ [m0] |
|---|---|---|---|---|
| **$MAEuI_3$** | 0.44/1.5 | 0.53/1.6 | 0.25/1.8 | 0.41/1.63 |
| **$MADyI_3$** | 0.47/0.51 | 0.43/0.85 | 0.27/2.3 | 0.39/1.22 |
| **$MaTmI_3$** | 0.42/1.6 | 0.35/2.4 | 0.30/-3.6 | 0.36/1.73 |
| **$MAYbI_3$** | 0.35/2.4 | 0.31/4.1 | 0.23/2.0 | 0.3/2.83 |

## Calculated Band gaps for U=5:

Eu is 3.34 eV. Dy=3.63,Tm=3.14,Yb=2.93)