Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Effect of Water Molecules on Chemical Stability of $MAGeI_3$ Perovskite Explored from Theoretical View

Ping-Ping Sun, Wei-Jie Chi, Ze-Sheng Li *

Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Key Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, School of Chemistry, Beijing Institute of Technology, Beijing 100081, China

* Corresponding author at: 5 South Zhongguancun Street Haidian Zone, Beijing 100081, China. Tel.: +86 10 68918670; fax: +86 10 68918670

E-mail: zeshengli@bit.edu.cn.

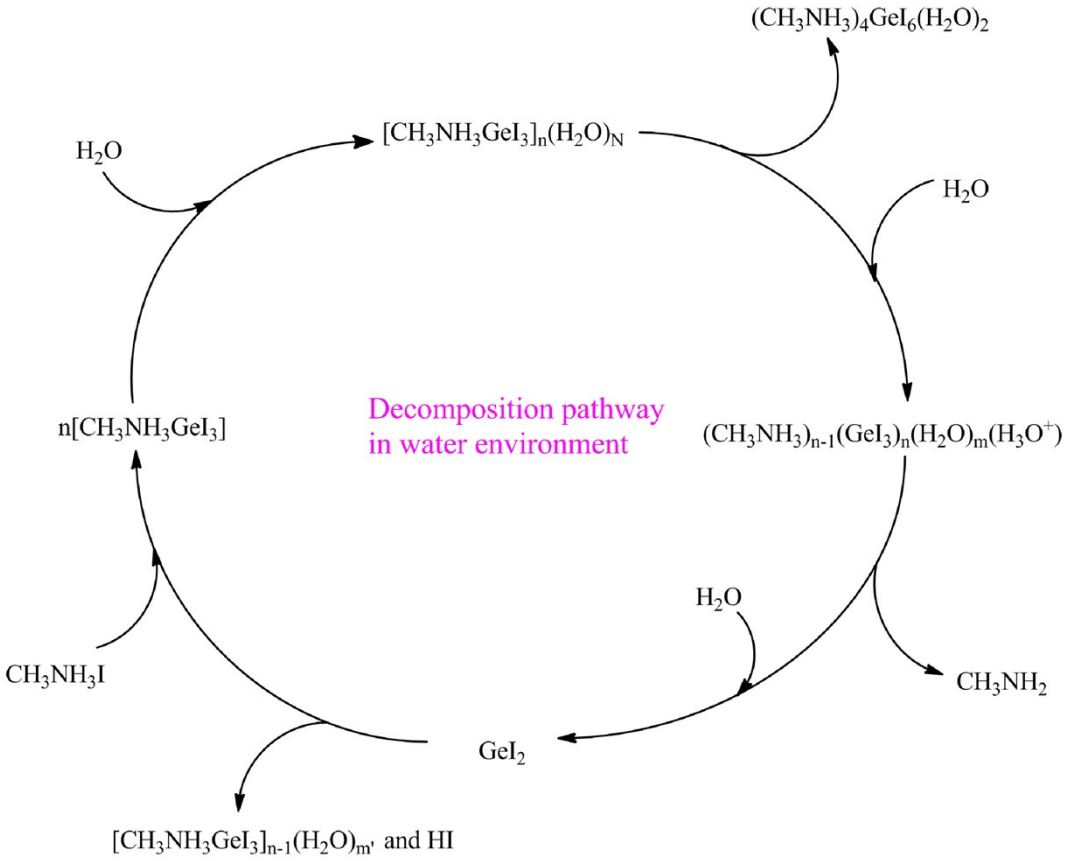

Figure S1. The possible degradation mechanism for $MAGeI_3$ perovskite under humidity exposure.

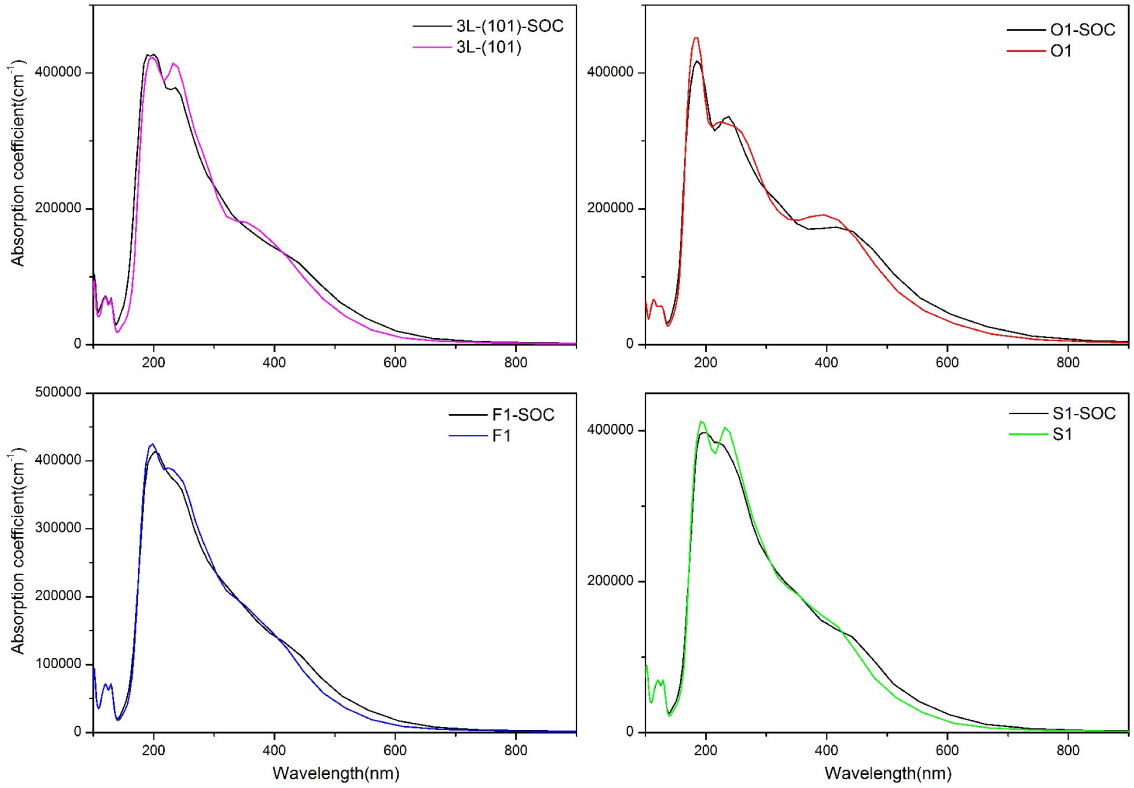

Figure S2. Optical absorption spectra of the clean (101) surface, O1, F1 and S1 structures calculated with different methods. The black lines are calculated at PBE-SOC method and the color lines are calculated at PBE method. It is clear to see that SOC has rather a weak effect on the absorption spectra, which only shows a slightly higher absorption in the range of 450 - 700 nm and a weaker absorption in the range of 180 – 450 nm. It also shows the same variation trend and conclusion as the main body shows.

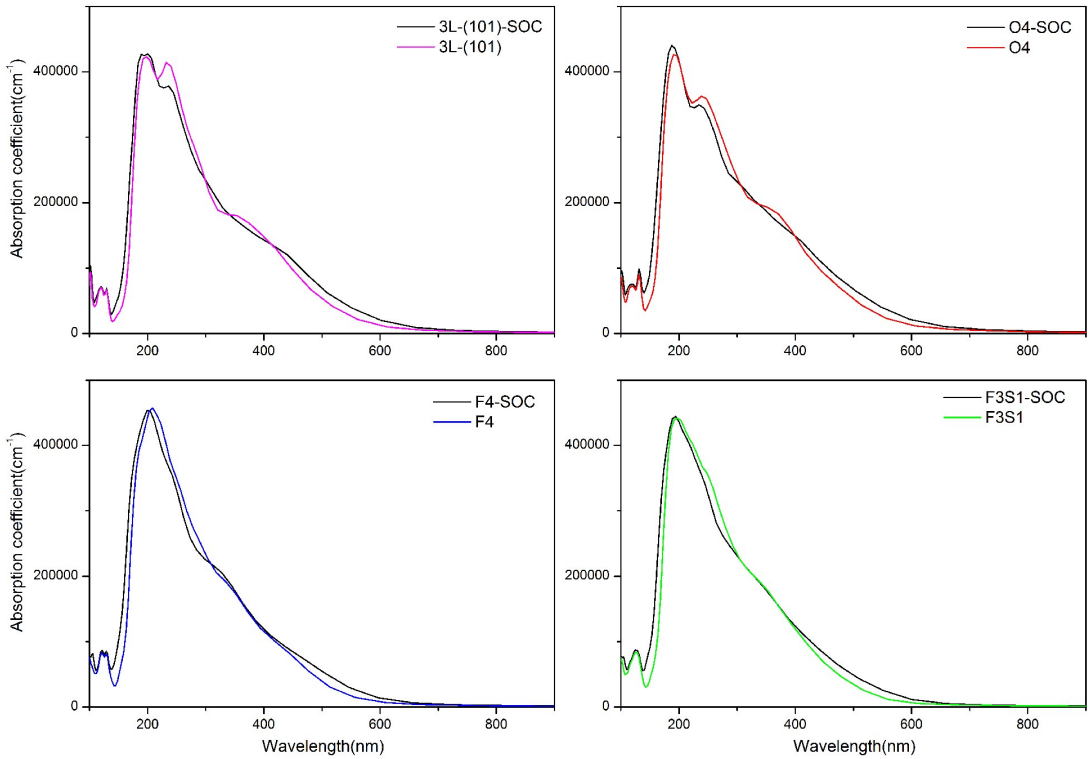

Figure S3. Optical absorption spectra of the clean (101) surface, O4, F4 and F3S1 structures calculated with different methods. The black lines are calculated at PBE-SOC method and the color lines are calculated at PBE method. Clearly, SOC has rather a weak effect on the absorption spectra where the black and the color lines overlap with each other approximately in the four systems.

Table S1. The calculated surface energies γ of Miller indices (001), (010), (011), (100), (101), (110), (111) surfaces of R3m phase $MAGeI_3$ perovskite.

Surface slab	Surface energy/(eV/Å^2·10^{-2})
(001)	5.902
(010)	6.493
(011)	6.627
(100)	6.571
(101)	5.248
(110)	6.018
(111)	6.693

Table S2. The adsorption energies of the systems with H_2O molecules adsorbed in the O region.

N/H_2O	E_{ads}
1	-0.098
2	-0.111
3	-0.13
4	-0.151
5	-0.145
6	-0.268
7	-0.151
8	-0.208
9	-0.214

Table S3. The relative energy E_r with the increasing number of the H_2O molecules staying between regions O and F.

N/H_2O	E_r
1	-0.22
2	-0.35
3	-0.8
4	-0.49
5	-0.25
6	0.31
7	0.66
8	0.11
9	0.02