Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Theoretical prediction and design for chalcogenide-quantum-dot/TiO_2 heterojunctions for solar cell applications

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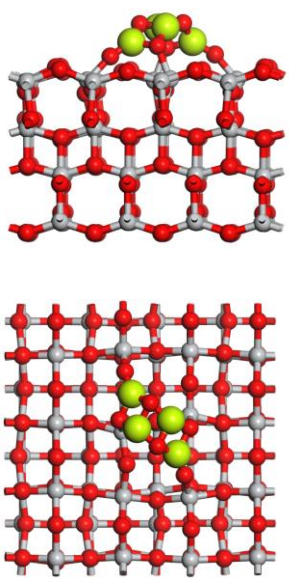
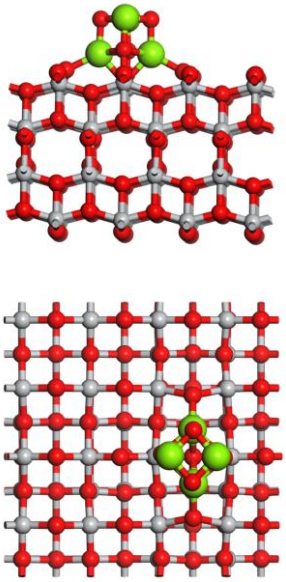


Be4O4/TiO_2(001)



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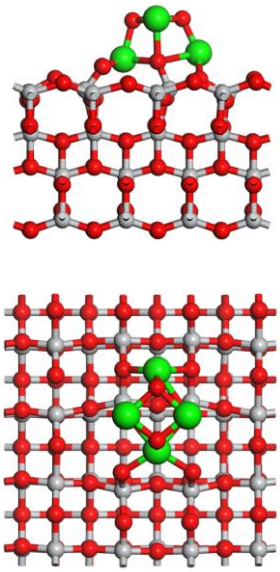

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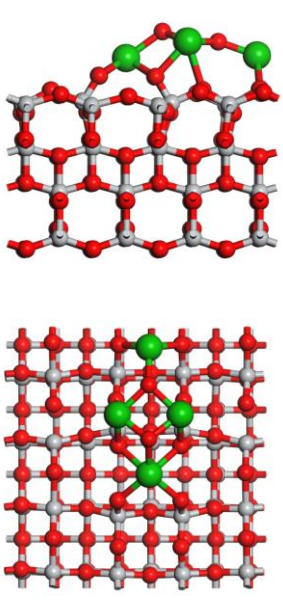

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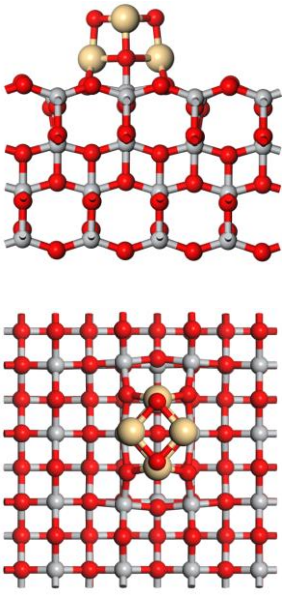

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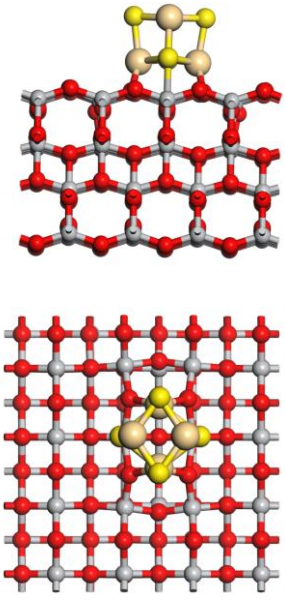

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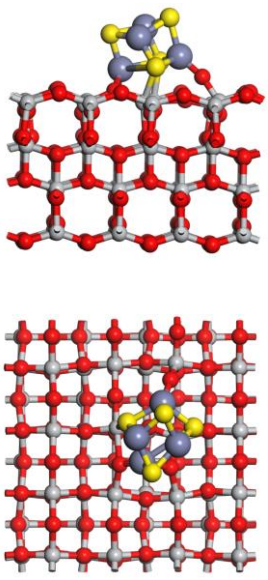

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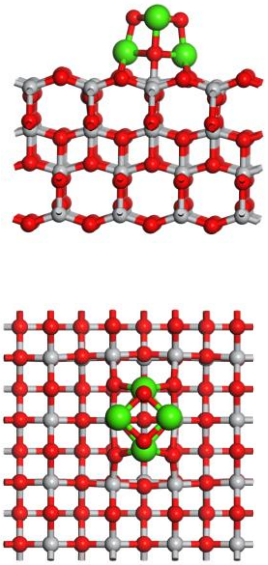

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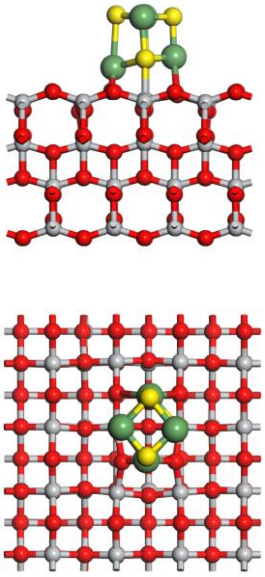

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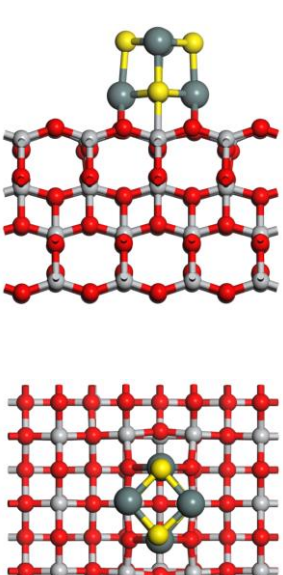

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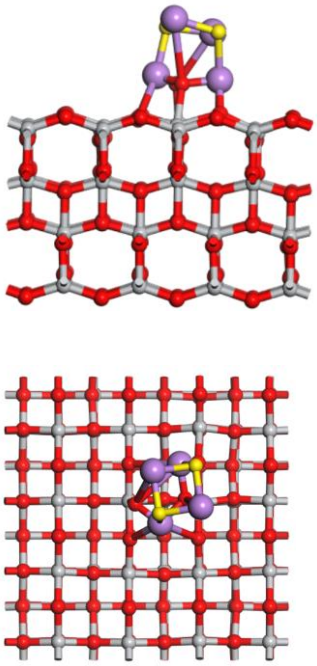

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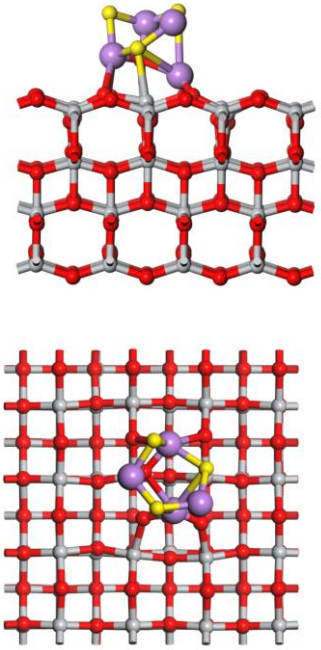

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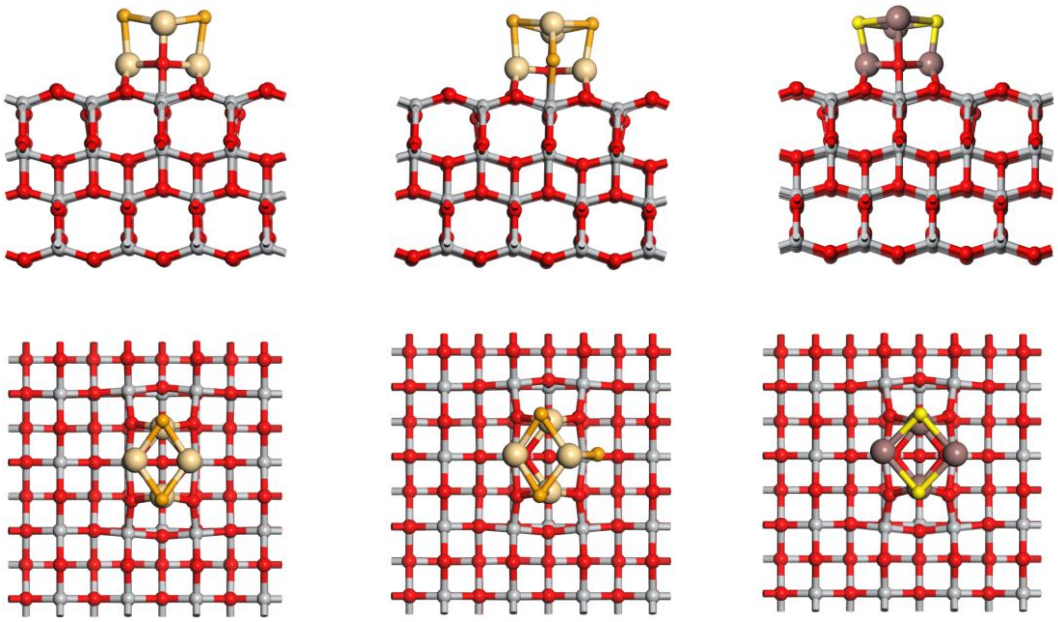

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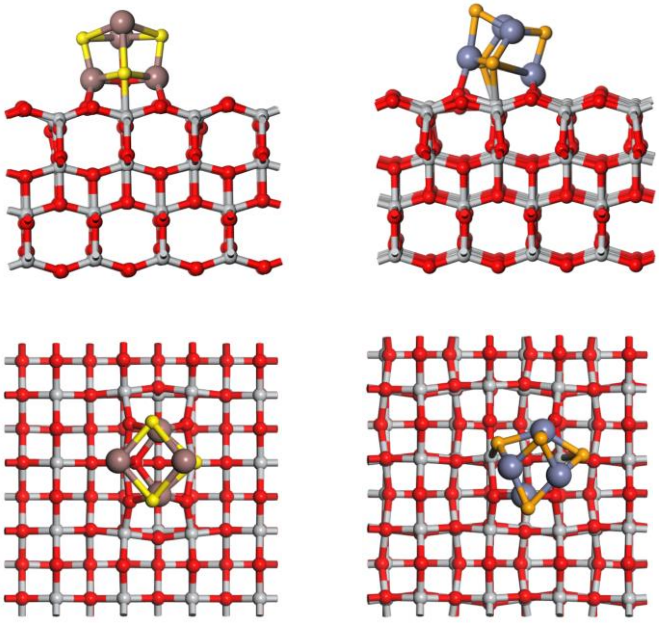
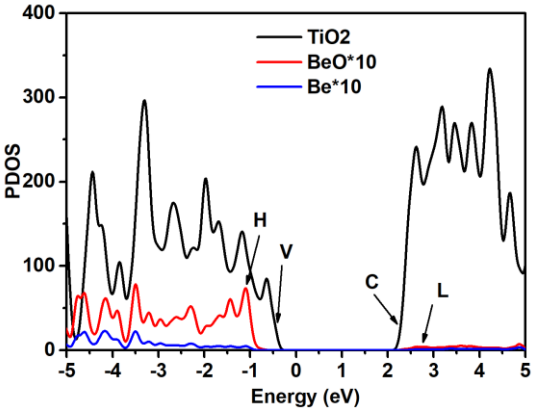


In4S3O/TiO_2(001) **Zn4Se4/TiO_2(001)**

Fig.S1 QD/TiO_2(001) Optimized structure



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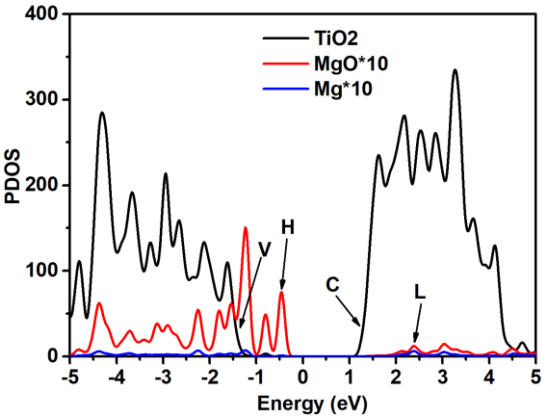

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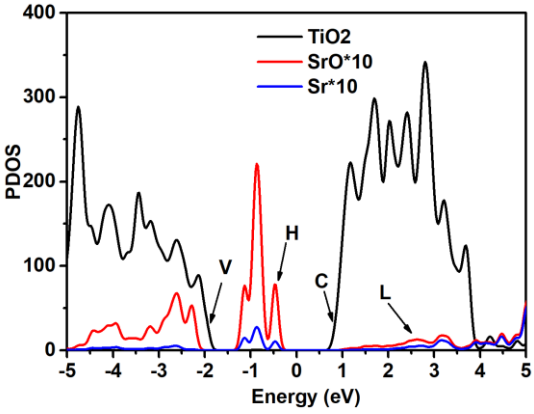

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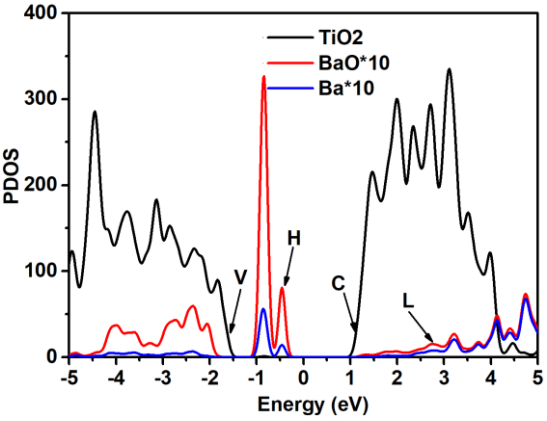

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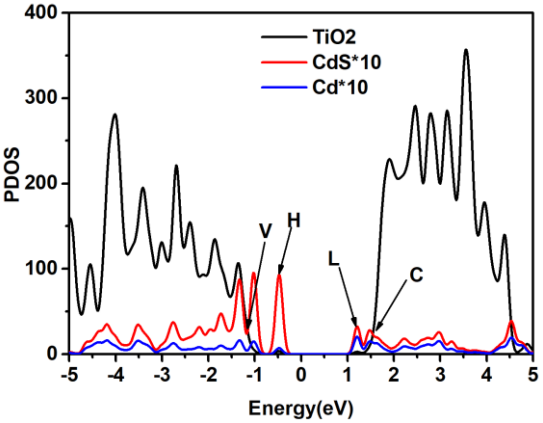

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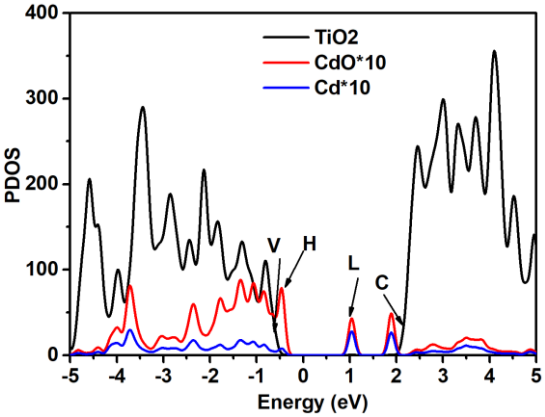

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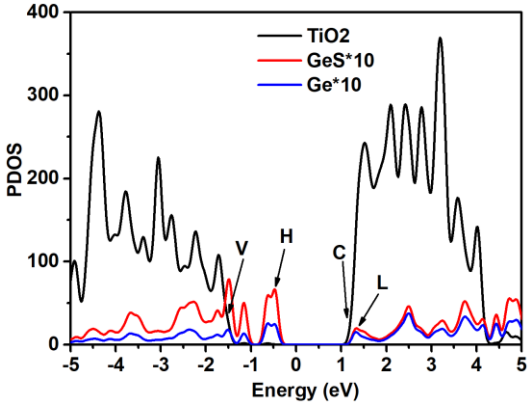

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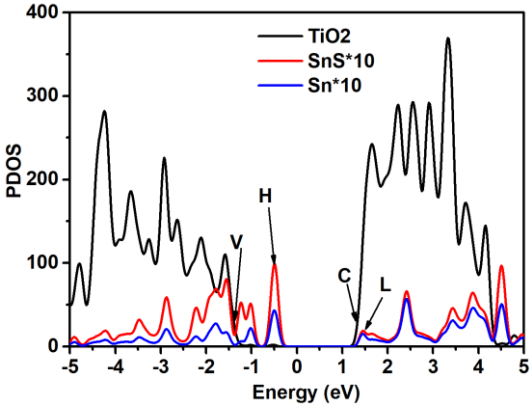

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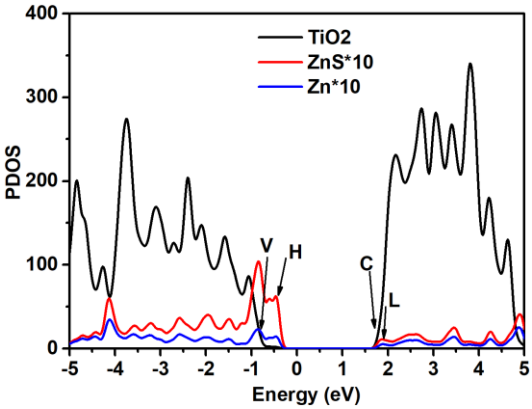

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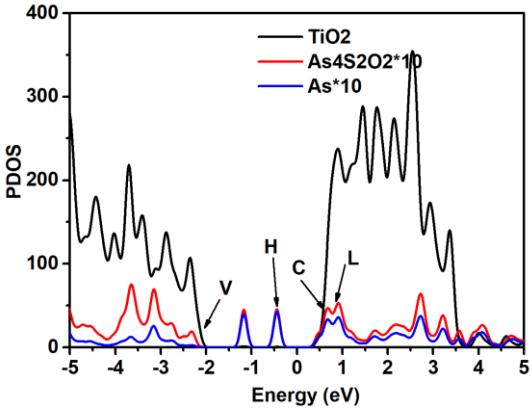

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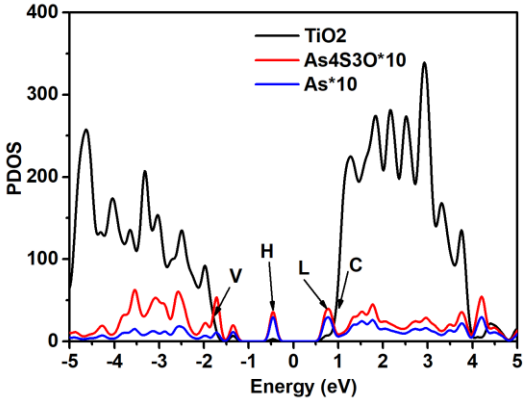

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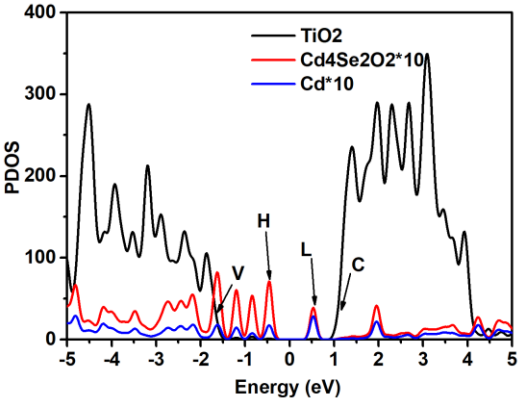

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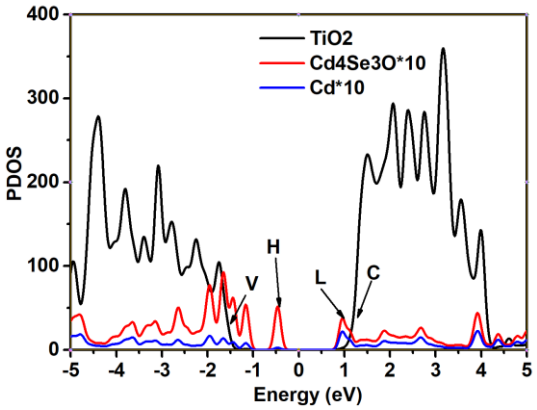

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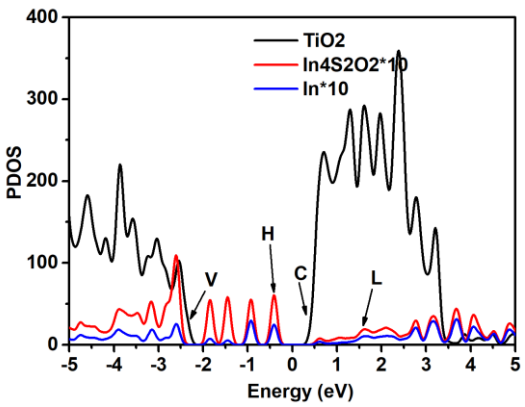

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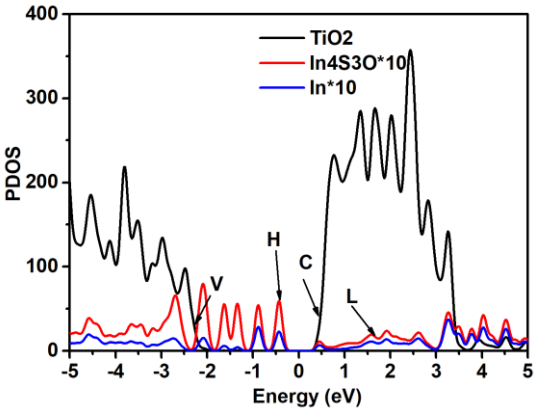

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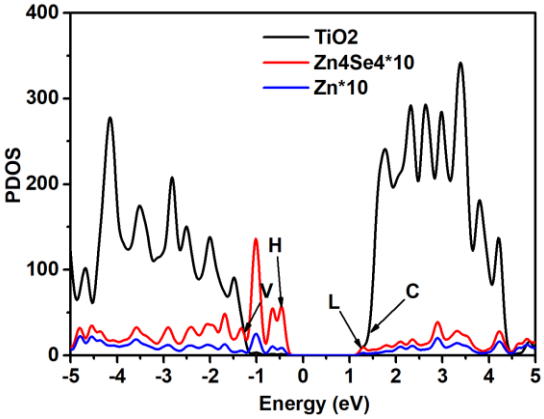

PDOS of Zn4Se4/TiO_2(001)

Fig.S2. Partial density of states

	A1	A2	A1/A2
Be4O4/TiO2	3.35E-07	603.72	5.55E-10
Cd4O4/TiO2	2.22	603.71	3.68E-03
Mg4O4/TiO2	5.28	607.82	8.69E-03
Ba4O4/TiO2	8.40	604.88	1.39E-02
Ca4O4/TiO2	9.10	601.88	1.51E-02
Sr4O4/TiO2	9.35	602.02	1.55E-02
Zn4S4/TiO2	10.95	604.01	1.81E-02
Cd4Se4/TiO2	12.90	604.95	2.13E-02
Cd4S4/TiO2	13.96	603.61	2.31E-02
Ge4S4/TiO2	26.70	604.12	4.42E-02
Sn4S4/TiO2	27.22	604.44	4.50E-02
In4S4/TiO2	29.77	603.90	4.93E-02
As4S4/TiO2	48.46	604.45	8.02E-02

Table S1. Effective photoexcitation intensities of different QD/TiO2(001) adsorption systems

	gap(eV)	wave length of gap (nm)	LUMO-HOMO (eV)	wave length of LUMO-HOMO (nm)	HOMO-VBM (eV)	LUMO-CBM (ev)
pure TiO_2	2.87	433				
Be4O4@TiO2	2.76	450	3.71	335	-0.67	0.28
Zn4S4@TiO2	2.27	548	2.33	533	0.45	0.06
Cd4Se4@TiO2	2.14	581	2.14	581	0.33	-0.16
Sn4S4@TiO2	1.83	679	1.94	641	0.92	0.11
Mg4O4@TiO2	1.74	714	2.82	441	0.93	1.08
Ge4S4@TiO2	1.70	731	1.80	691	0.99	0.10
Cd4S4@TiO2	1.65	753	1.65	753	0.71	-0.39
Ba4O4@TiO2	1.59	782	3.19	390	1.14	1.60
Ca4O4@TiO2	1.54	807	3.49	356	1.21	1.95
Cd4O4@TiO2	1.50	829	1.50	829	0.14	-1.11
Sr4O4@TiO2	1.30	956	3.10	401	1.44	1.80
In4S4@TiO2	0.87	1429	0.87	1429	1.72	-0.16
As4S4@TiO2	0.79	1573	0.79	1573	1.73	-0.24

Table S2. The PDOS information of the adsorption system is, in turn, the band gap, the wavelength corresponding to the band gap, the LUMO-HOMO energy level, the HOMO-VBM energy level, and the LUMO-CBM energy level.

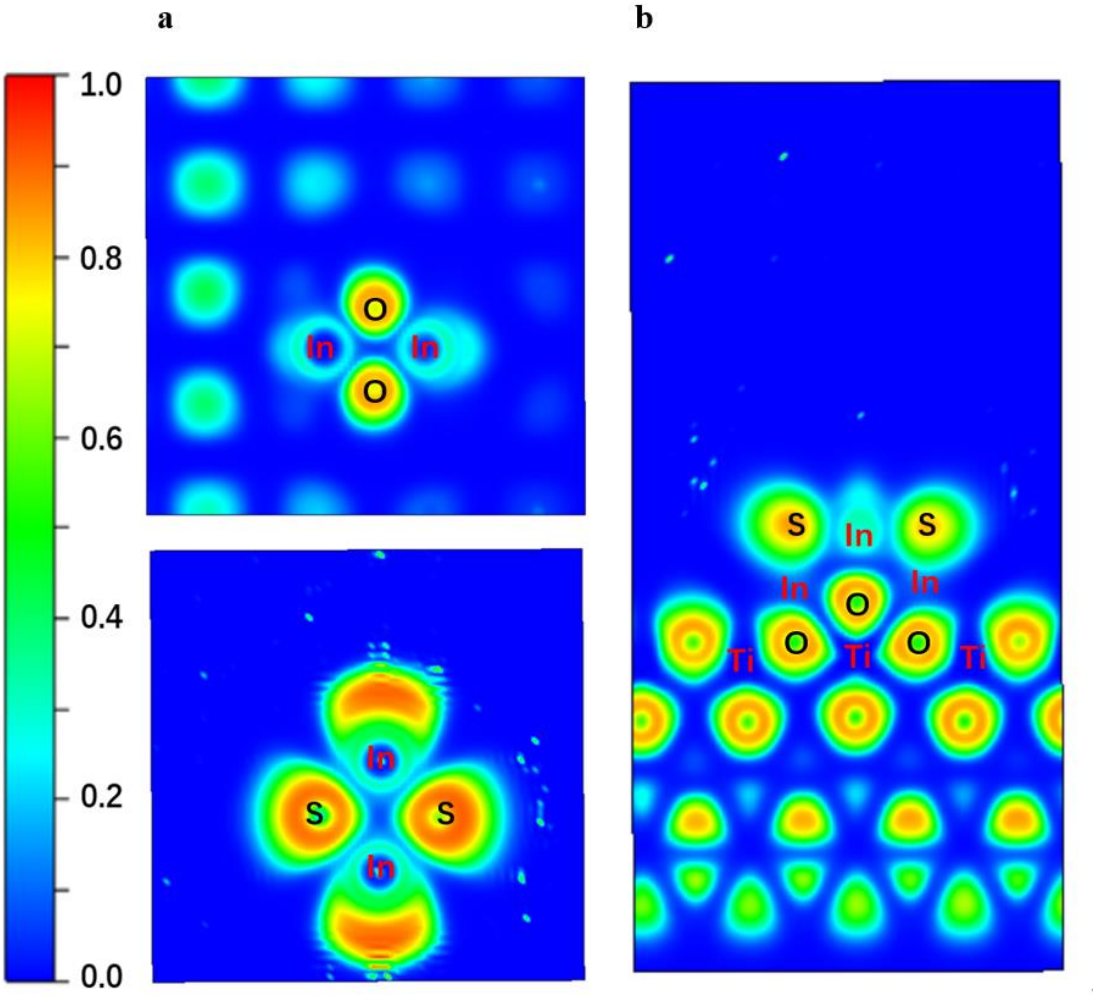

Fig.S3. ELF plots of $In_4S_2O_2/TiO_2$, projected on the: (a) (001) plane, (b) (100) plane.

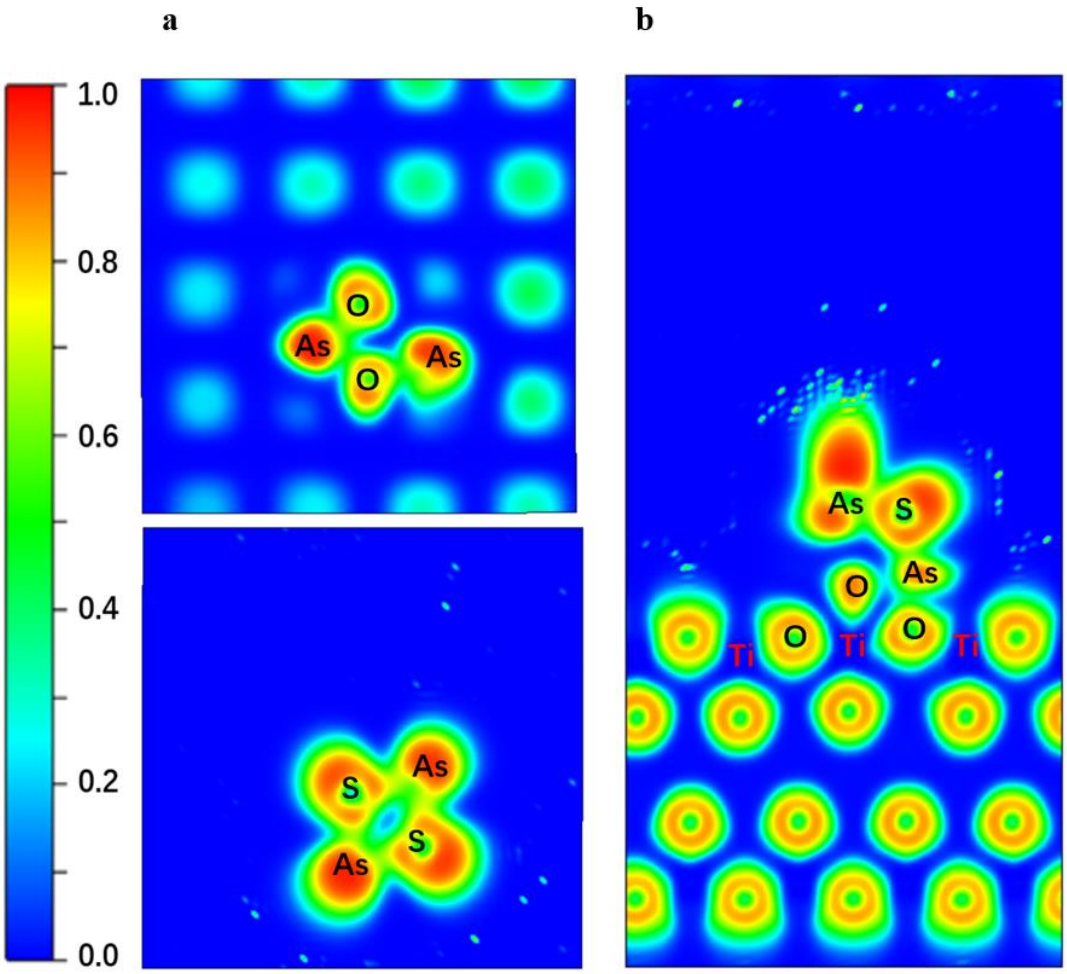

Fig.S4 ELF plots of $As_4S_2O_2/TiO_2$, projected on the: (a) (001) plane, (b) (100) plane.