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

SUPPLEMENTARY INFORMATION FOR

Unraveling the Origin of High Photocatalytic Properties of Earth-abundant TiO_2/FeS_2 Heterojunction: Insights from First-Principles Density Functional Theory

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Figure S1: The projected density of states (PDOS) of bulk FeS_2 calculated at different effective U-values. The bandgap (E_g) predicted at each U value is displayed on each figure in blue.

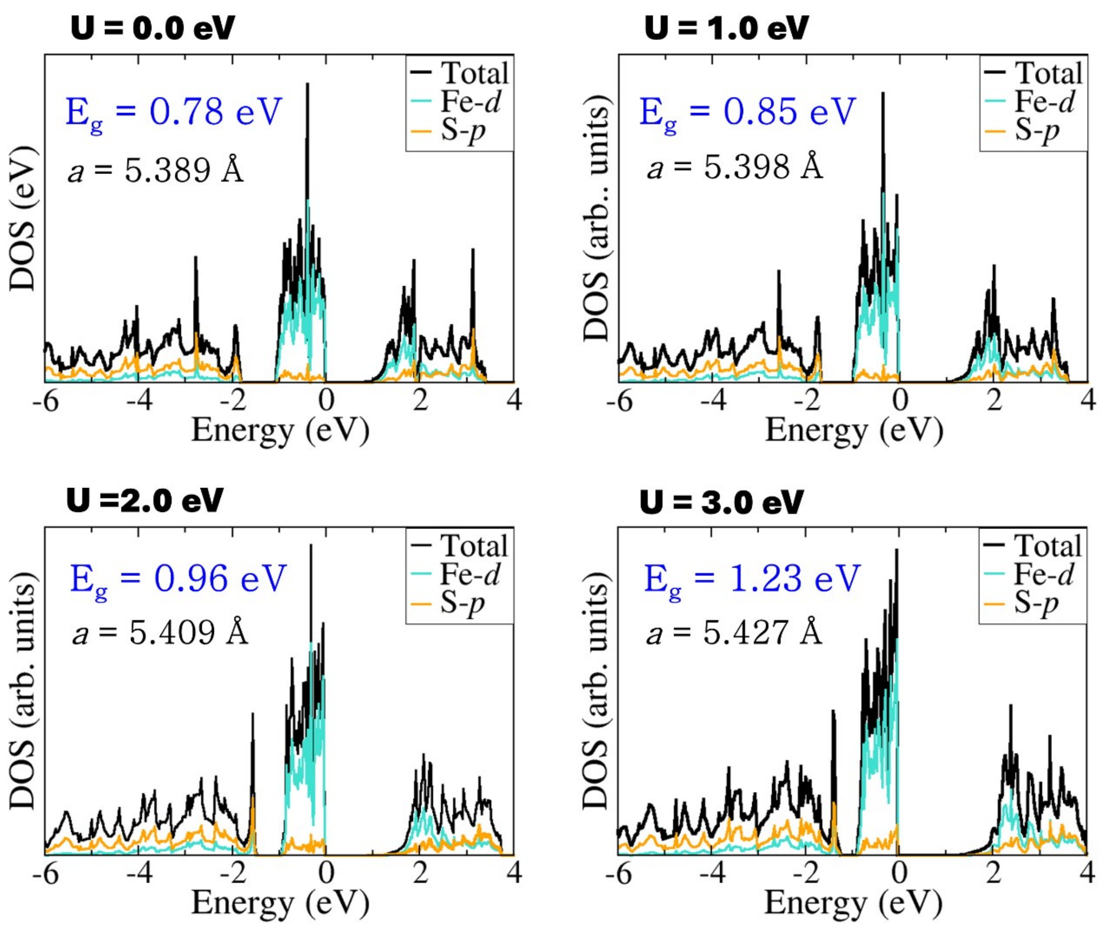

Figure S2: The projected density of states (PDOS) of bulk anatase TiO_2 calculated at different effective U-values. The bandgap (E_g) predicted at each U value is displayed on each figure in blue.

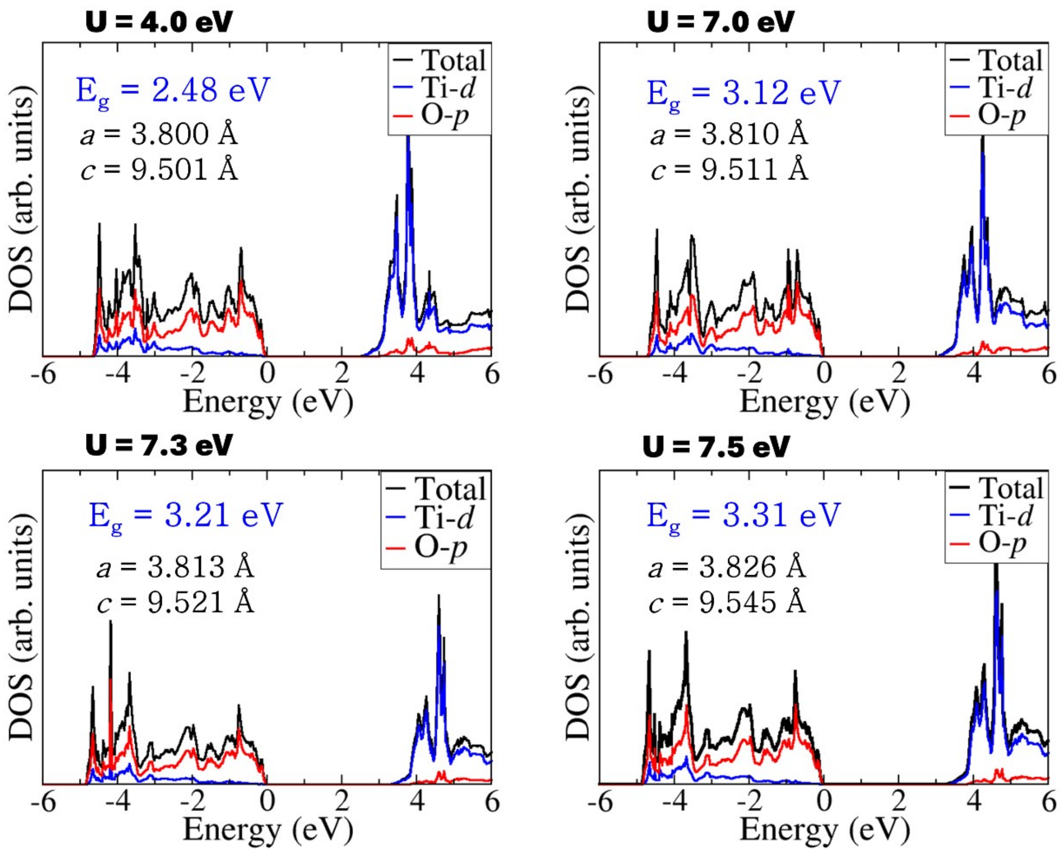

Table S1: Bader charge analysis results $FeS_2(100)$-$TiO_2(001)$ heterojunction. The sum of the charges of FeS_2 ions (Fe and S) is 0.8734 e^-, whereas that of TiO_2 ions (Ti and O) is -0.8733 e^-. This indicates that a total charge of 0.87 e^- is transferred from the $FeS_2(100)$ layers to the top of the $TiO_2(001)$ layer.

Element	**Bader charge (e^-)**
Fe	0.9479
Fe	1.0418
Fe	0.9039
Fe	0.9069
Fe	0.9002
Fe	0.9012
Fe	0.9317
Fe	0.9093
Fe	0.8955
Fe	0.9312
Fe	0.8982
Fe	0.9041
Fe	0.9116
Fe	0.9075
Fe	0.9298
Fe	0.9021
Fe	0.9749
Fe	0.9191
Fe	0.9052
Fe	0.9
Fe	0.9038
Fe	0.8994
Fe	0.8986
Fe	0.9341
Fe	0.6347
Fe	0.9468
Fe	0.9015
Fe	0.908
Fe	0.906
Fe	0.9117
Fe	0.9025
Fe	0.9284
S	-0.5219
S	-0.4944
S	-0.4639
S	-0.4935
S	-0.454
S	-0.4512
S	-0.485

S	-0.4234
S	-0.4401
S	-0.462
S	-0.4298
S	-0.3987
S	-0.4894
S	-0.5196
S	-0.4272
S	-0.4618
S	-0.4671
S	1.0116
S	-0.5367
S	-0.481
S	-0.4313
S	-0.4292
S	-0.4975
S	-0.4837
S	-0.4525
S	-0.44
S	-0.4125
S	-0.4287
S	-0.5085
S	-0.496
S	-0.436
S	-0.4322
S	-0.5089
S	-0.5864
S	-0.5294
S	-0.4897
S	-0.3685
S	-0.3881
S	-0.4686
S	-0.4687
S	-0.4899
S	-0.4572
S	-0.4434
S	-0.4193
S	-0.4956
S	-0.5059
S	-0.4268
S	-0.4259
S	-0.6423
S	-0.3239
S	-0.4919
S	-0.519

S	-0.435
S	-0.4007
S	-0.4539
S	-0.4636
S	-0.4471
S	-0.471
S	-0.4124
S	-0.4258
S	-0.5297
S	-0.519
S	-0.4548
S	-0.4246
Ti	2.7581
Ti	2.7536
Ti	2.8086
Ti	2.7026
Ti	2.7359
Ti	2.7644
Ti	2.7585
Ti	2.7695
Ti	2.7562
Ti	2.794
Ti	2.7755
Ti	2.7167
Ti	2.7559
Ti	2.7608
Ti	2.7679
Ti	2.7392
Ti	2.733
Ti	2.7654
Ti	2.7713
Ti	2.711
Ti	2.7467
Ti	2.7556
Ti	2.7843
Ti	2.7134
Ti	2.7609
Ti	2.7805
Ti	2.7939
Ti	2.7407
Ti	2.772
Ti	2.7589
Ti	2.7807
Ti	2.7335
Ti	2.7439

Ti	2.7615
Ti	2.7734
Ti	2.5465
O	-1.3342
O	-1.4004
O	-1.3991
O	-1.408
O	-1.3744
O	-1.4294
O	-1.435
O	-1.3552
O	-1.3206
O	-1.3984
O	-1.3925
O	-1.387
O	-1.3781
O	-1.4105
O	-1.3967
O	-1.3577
O	-1.3323
O	-1.4175
O	-1.4065
O	-1.3834
O	-1.3952
O	-1.4127
O	-1.4108
O	-1.2295
O	-1.3331
O	-1.4029
O	-1.404
O	-1.3864
O	-1.3764
O	-1.4166
O	-1.3796
O	-1.2907
O	-1.3229
O	-1.4098
O	-1.3885
O	-1.3914
O	-1.3842
O	-1.4169
O	-1.3858
O	-1.2853
O	-1.3323
O	-1.4096

O	-1.3791
O	-1.3979
O	-1.3807
O	-1.4043
O	-1.4129
O	-1.2902
O	-1.3322
O	-1.4102
O	-1.3978
O	-1.3874
O	-1.3945
O	-1.4106
O	-1.399
O	-1.3477
O	-1.3341
O	-1.4108
O	-1.4052
O	-1.3965
O	-1.3821
O	-1.4056
O	-1.3958
O	-1.8931
O	-1.337
O	-1.4079
O	-1.3824
O	-1.4052
O	-1.3858
O	-1.3891
O	-1.4152
O	-1.346