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

Supporting Information

Optical properties of in-plane chemically ordered i-MAX structures

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$(Mo_{2/3}Sc_{1/3})_2AlC$

Atomic Charge Difference

Atom	Charge
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Sc	-1.3821
Mo	4.5684
Mo	4.5775
Mo	4.5775
Mo	4.5684
Mo	4.5684
Mo	4.5777
Mo	4.5775
Mo	4.5684
Mo	4.5684
Mo	4.5775
Mo	4.5775
Mo	4.5684
Mo	4.5684
Mo	4.5775
Mo	4.5775
Mo	4.5684
Al	-0.1754
Al	-0.1756
Al	-0.1754
Al	-0.1755
Al	-0.0661
Al	-0.0875
Al	-0.0875
Al	-0.0661
Al	-0.0661
Al	-0.0875
Al	-0.0875
Al	-0.0661
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5390
C	1.5970
C	1.5970
C	1.5971
C	1.5971

$(Mo_{2/3}Sc_{1/3})_2GaC$

Atomic Charge Difference

Atom	Charge
Sc	-5.4489
Sc	-5.4489
Sc	-5.1945
Sc	-5.1945
Sc	-5.5680
Sc	-5.5680
Sc	-5.4631
Sc	-5.4631
Mo	-8.2597
Mo	-8.2597
Mo	-7.6266
Mo	-7.6266
Mo	-8.2597
Mo	-8.2597
Mo	-7.6266
Mo	-7.6266
Mo	-7.2978
Mo	-7.2978
Mo	-4.0580
Mo	-4.0580
Mo	-7.2978
Mo	-7.2978
Mo	-4.0580
Mo	-4.0580
Ga	-4.0632
Ga	-4.0632
Ga	-5.1200
Ga	-5.1200
Ga	-4.7202
Ga	-4.7202
Ga	-4.7202
Ga	-4.7202
Ga	-4.7475
Ga	-4.7475
Ga	-4.7475
Ga	-4.7475
C	-3.9475
C	-3.9497
C	-3.9475
C	-3.9497
C	-3.9440
C	-3.9488
C	-3.9440
C	-3.9488
C	-3.9390
C	-3.9479
C	-3.9478
C	-3.9495

$(Mo_{2/3}Sc_{1/3})_2InC$

Atomic Charge Difference

Atom	Charge
Sc	-1.4286
Sc	-1.4286
Sc	-0.7585
Sc	-0.7585
Sc	-1.7294
Sc	-1.7294
Sc	-1.6520
Sc	-1.6520
Mo	-1.8316
Mo	-1.8374
Mo	-1.4633
Mo	-1.4590
Mo	-1.8316
Mo	-1.8374
Mo	-1.4633
Mo	-1.4590
Mo	-1.0437
Mo	-1.0481
Mo	1.0976
Mo	1.1036
Mo	-1.0437
Mo	-1.0481
Mo	1.0976
Mo	1.1036
In	1.1882
In	1.1882
In	-0.6997
In	-0.6997
In	1.6737
In	1.6729
In	1.6729
In	1.6737
In	-0.7873
In	-0.7982
In	-0.7982
In	-0.7873
C	1.5917
C	1.5906
C	1.5916
C	1.5906
C	1.5944
C	1.5912
C	1.5944
C	1.5912
C	1.6105
C	1.6055
C	1.6090
C	1.6037

$(Mo_{2/3}Sc_{1/3})_2SnC$

Atomic Charge Difference

Atom	Charge
Sc	-1.6413
Sc	-1.6413
Sc	-1.6413
Sc	-1.6413
Sc	-1.6408
Sc	-1.6407
Sc	-1.6408
Sc	-1.6408
Mo	0.3765
Mo	0.3704
Mo	0.3704
Mo	0.3765
Mo	0.3765
Mo	0.3704
Mo	0.3704
Mo	0.3765
Mo	-1.2414
Mo	-1.2476
Mo	-1.2476
Mo	-1.2414
Mo	-1.2414
Mo	-1.2475
Mo	-1.2476
Mo	-1.2414
Sn	-0.2748
Sn	-0.2748
Sn	-0.9434
Sn	-0.9434
Sn	0.0064
Sn	-0.0180
Sn	-0.0180
Sn	0.0064
Sn	-1.0421
Sn	-1.0621
Sn	-1.0621
Sn	-1.0421
C	1.5901
C	1.5901
C	1.5901
C	1.5901
C	1.5821
C	1.5821
C	1.5821
C	1.5821
C	1.5846
C	1.5846
C	1.5813
C	1.5813

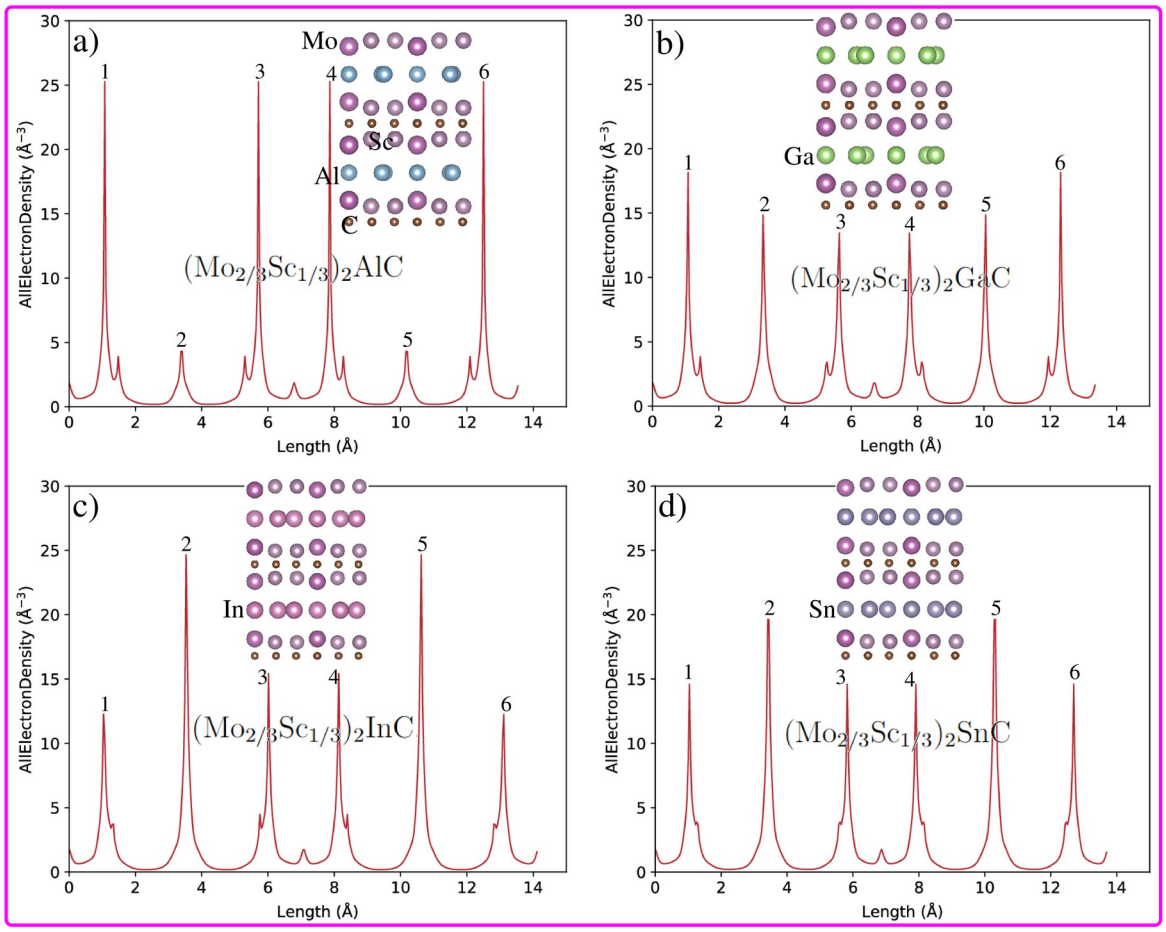

Figure S1: All electron density profile of the $(Mo_{2/3}Sc_{1/3})_2AlC$, $(Mo_{2/3}Sc_{1/3})_2GaC$, $(Mo_{2/3}Sc_{1/3})_2InC$, and $(Mo_{2/3}Sc_{1/3})_2ScC$ i-MAX structures. Note that the peaks are numbered.

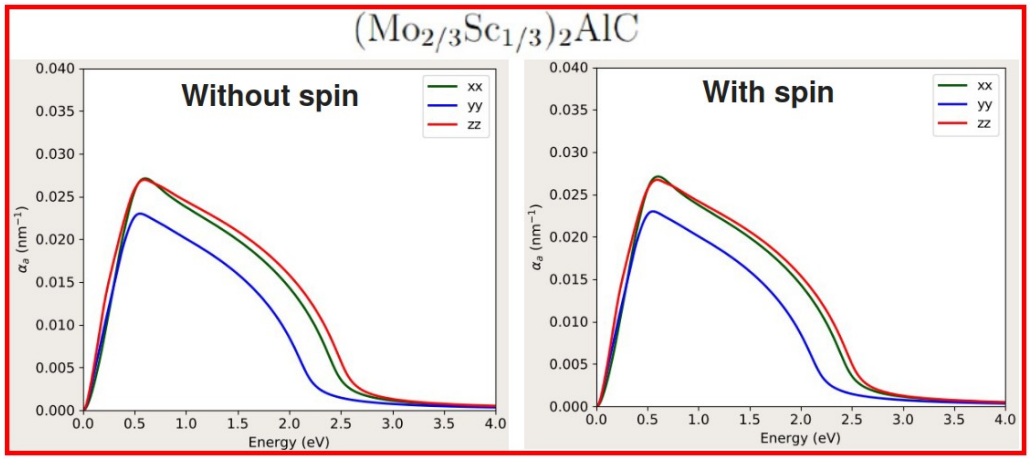

Figure S2: Comparing the photoabsorption spectra without and with spin.

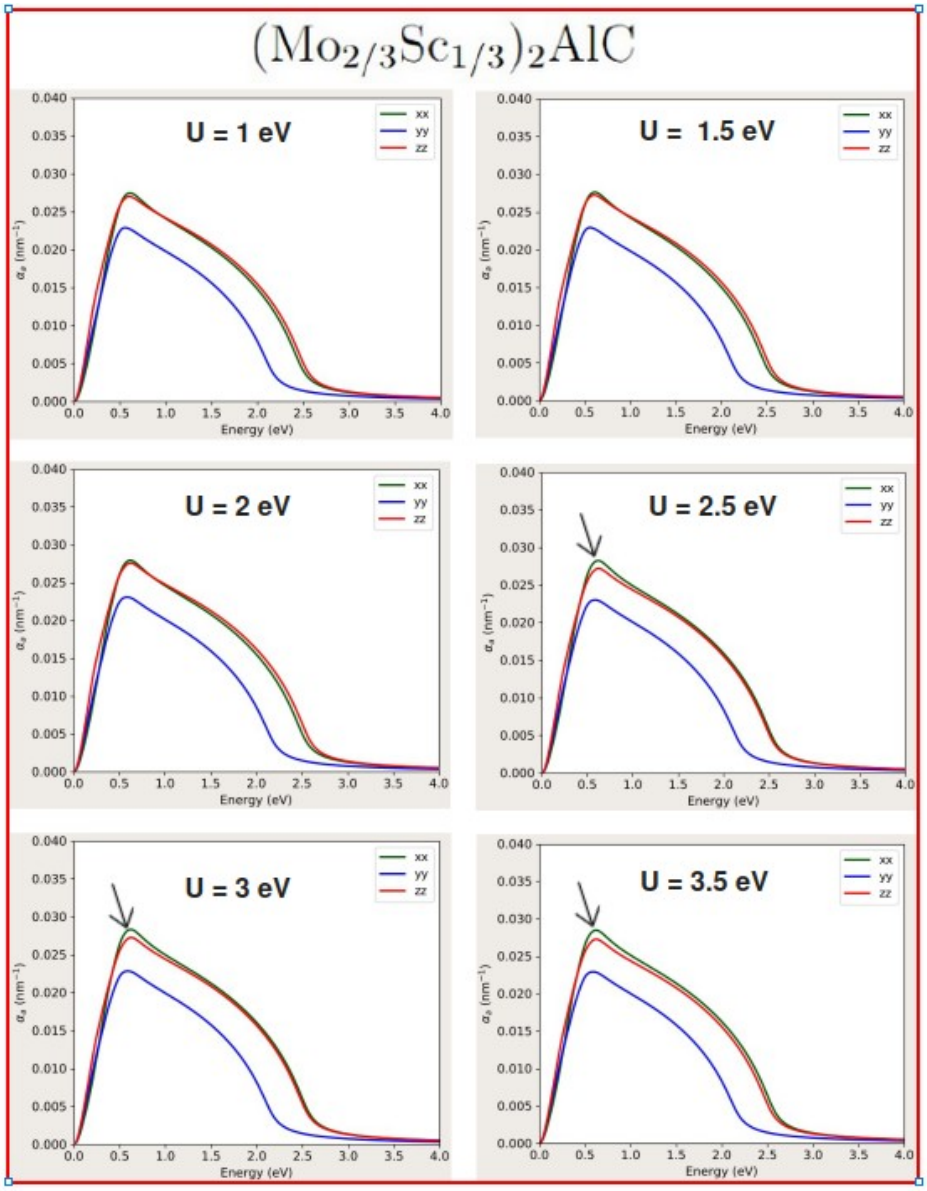

Figure S3: Photoabsorption spectra with Hubbard U parameter.

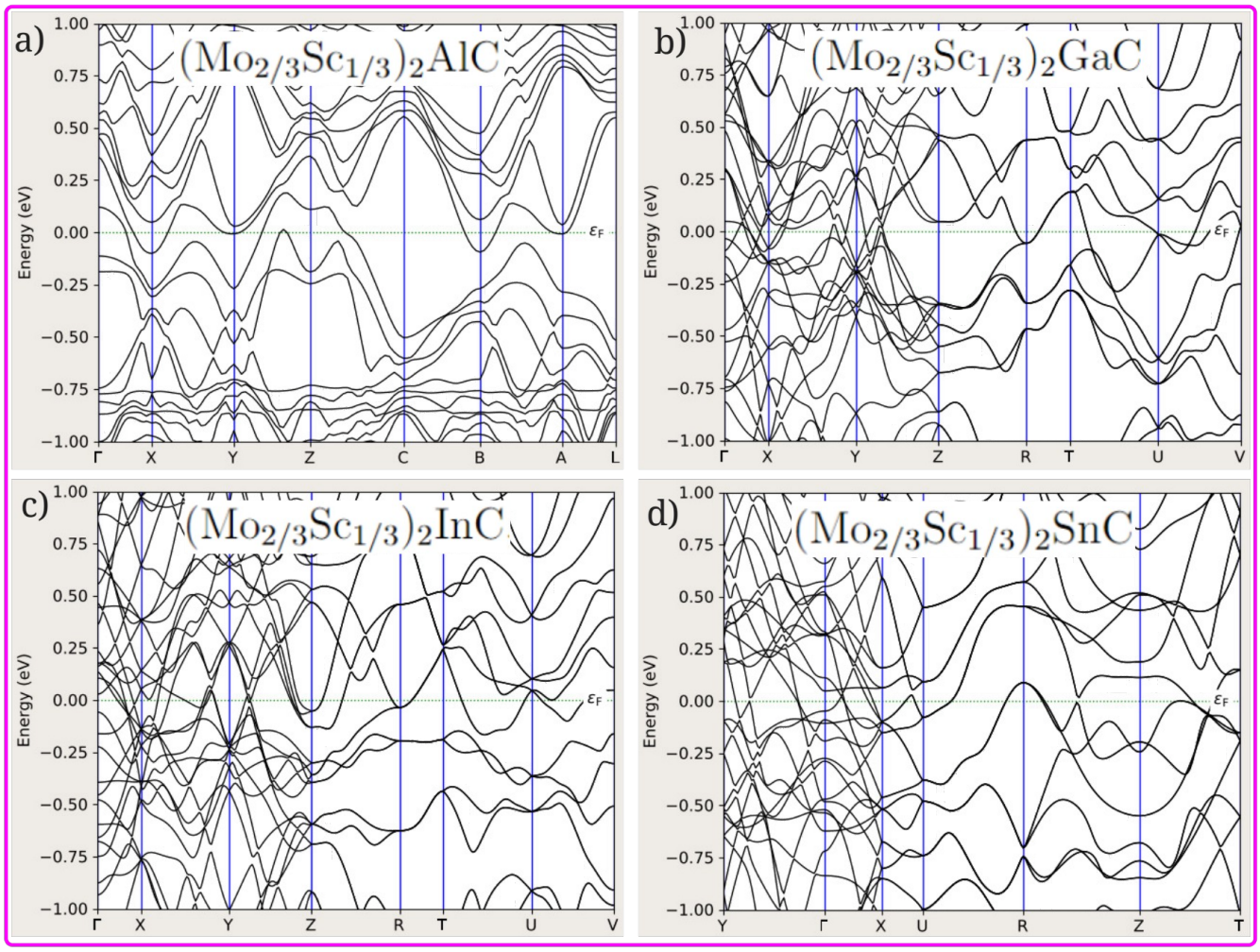

Figure S4: Band structure with HSE functional.