Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Two-dimensional multi-layer M_2CO_2 (M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: A first principles study

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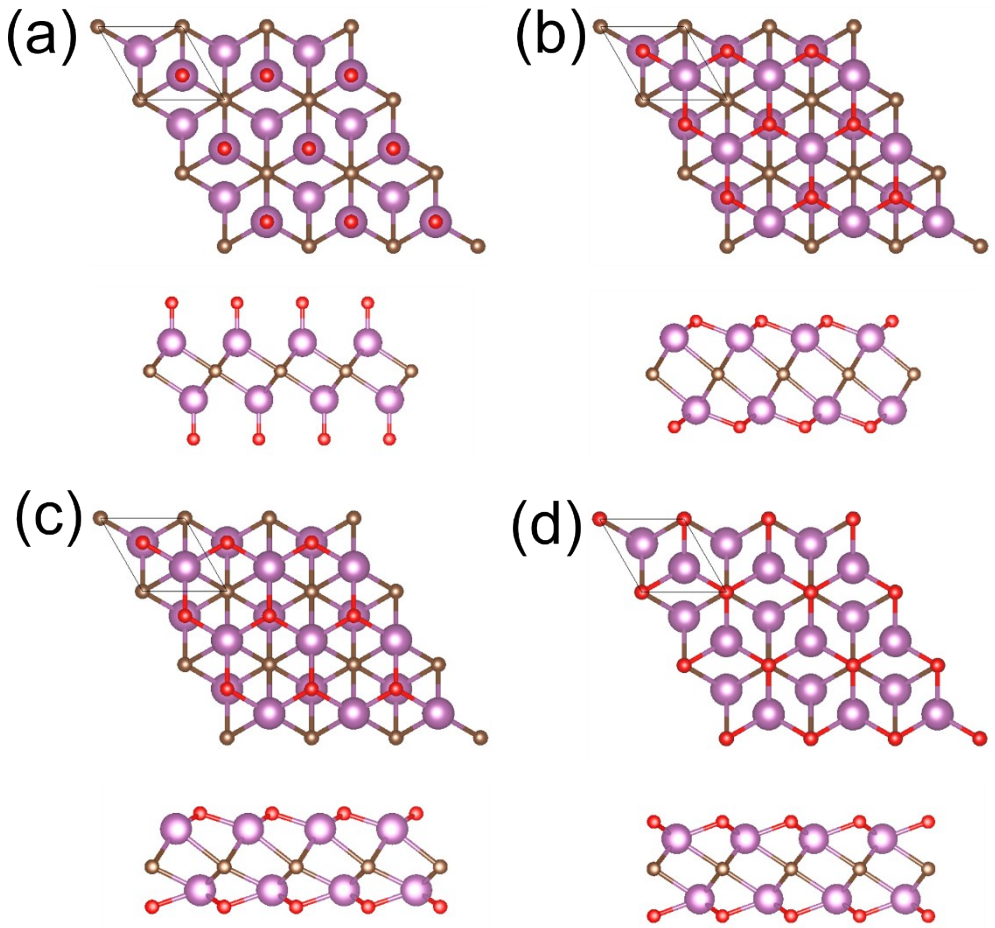

Figure S1. Geometry of the four models of M_2CO_2 (M = Sc, Zr, Hf): (a) Model 1, (b) Model 2, (c) Model 3, and (d) Model 4, respectively. The orchid, brown and red atoms represent metal, C and O atoms, respectively.

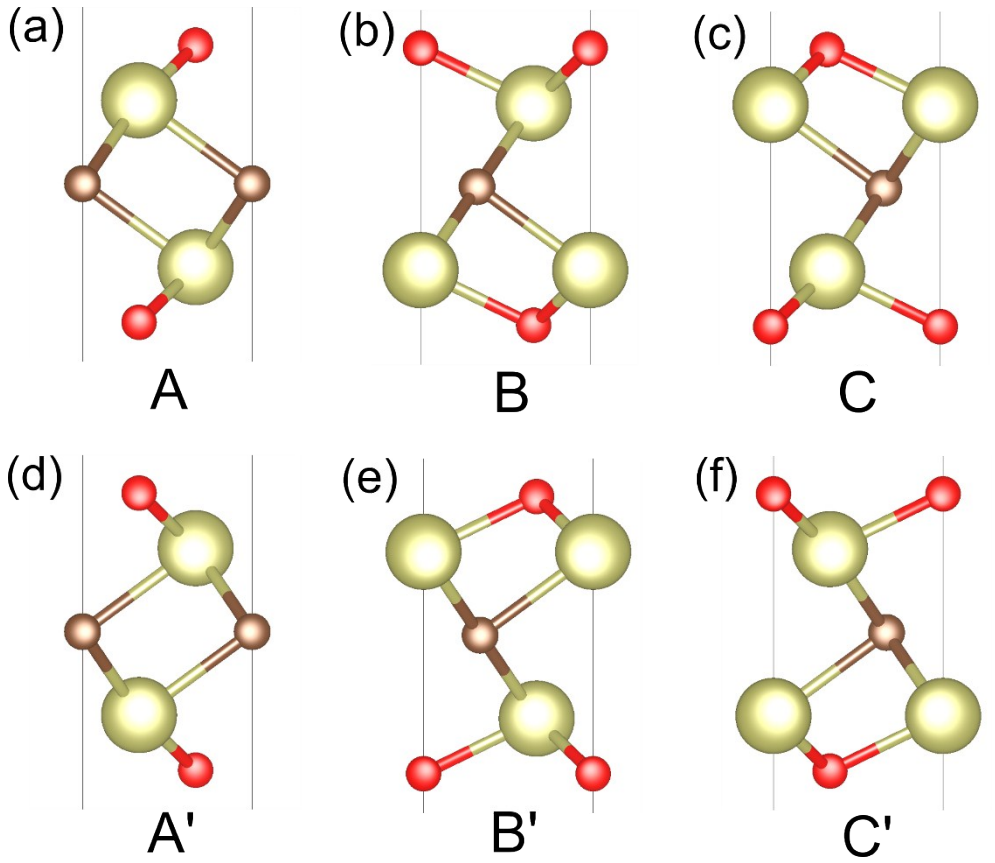

Figure S2. Different configurations for multilayer Zr_2CO_2 and Hf_2CO_2: (a) A, (b) B, (c) C, (d) A', (e) B', (f) C'.

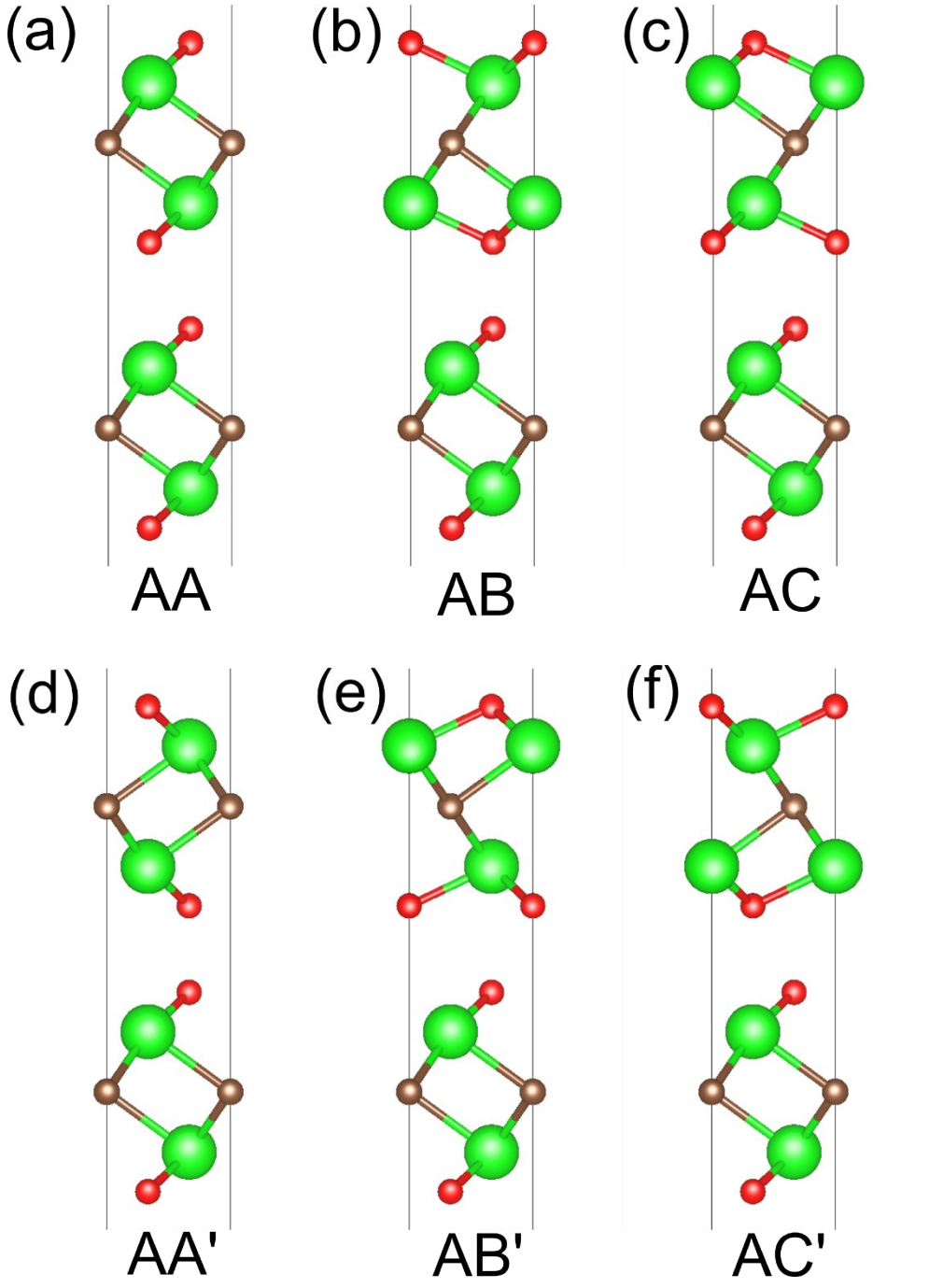

Figure S3. Different stacking configurations for bilayer Zr_2CO_2.

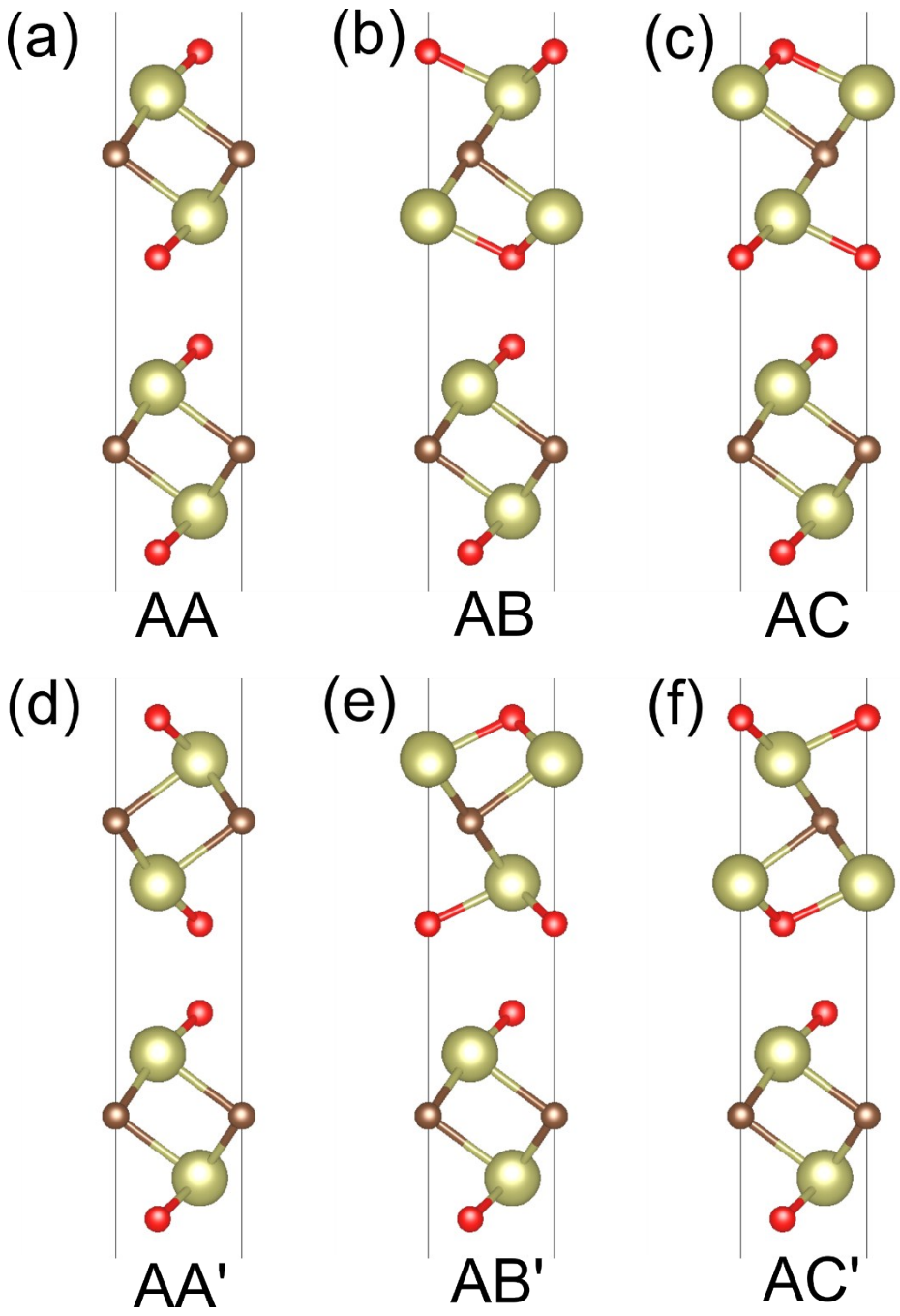

Figure S4. Different stacking configurations for bilayer Hf_2CO_2.

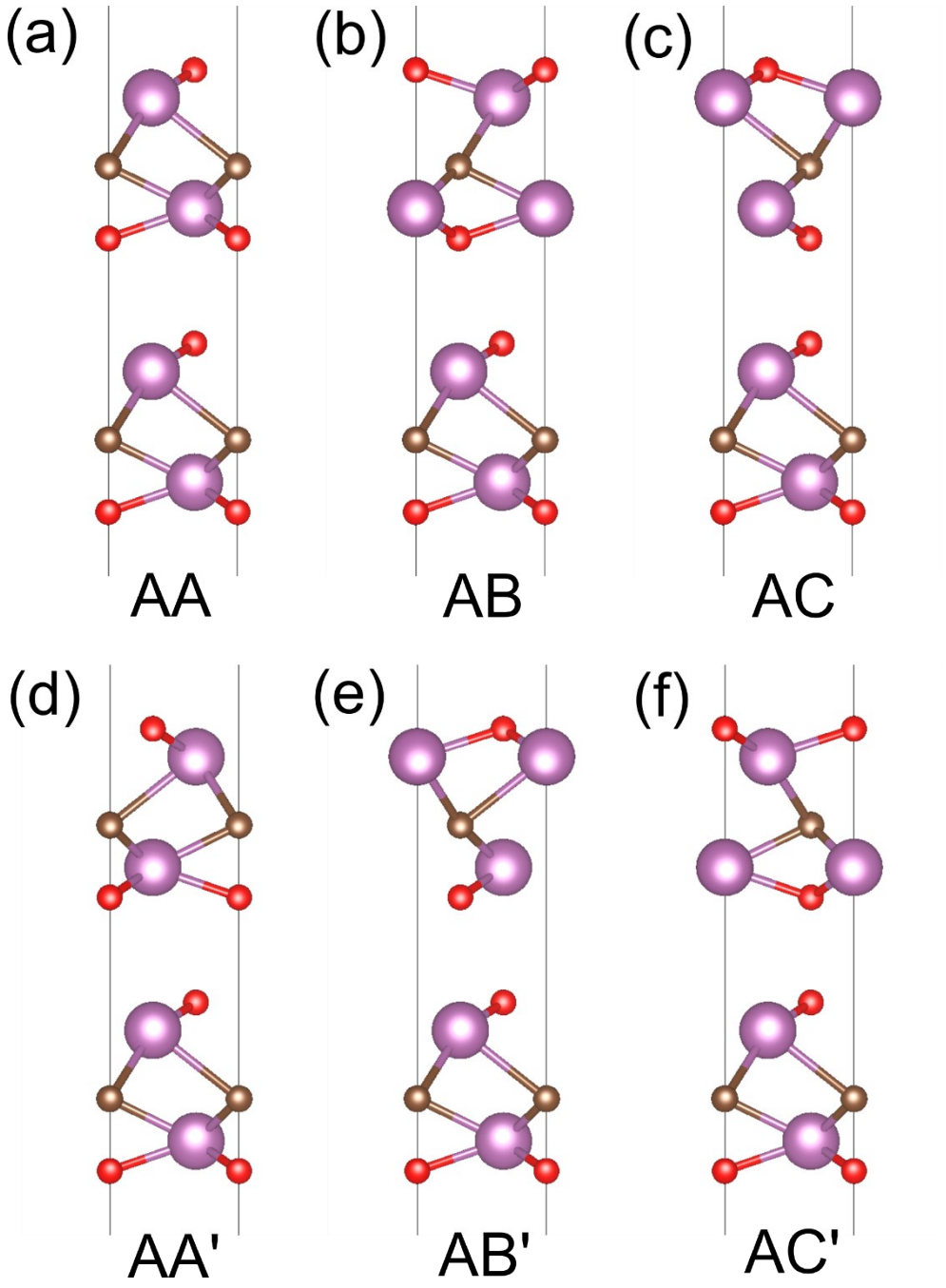

Figure S5. Different stacking configurations for bilayer UU Sc_2CO_2.

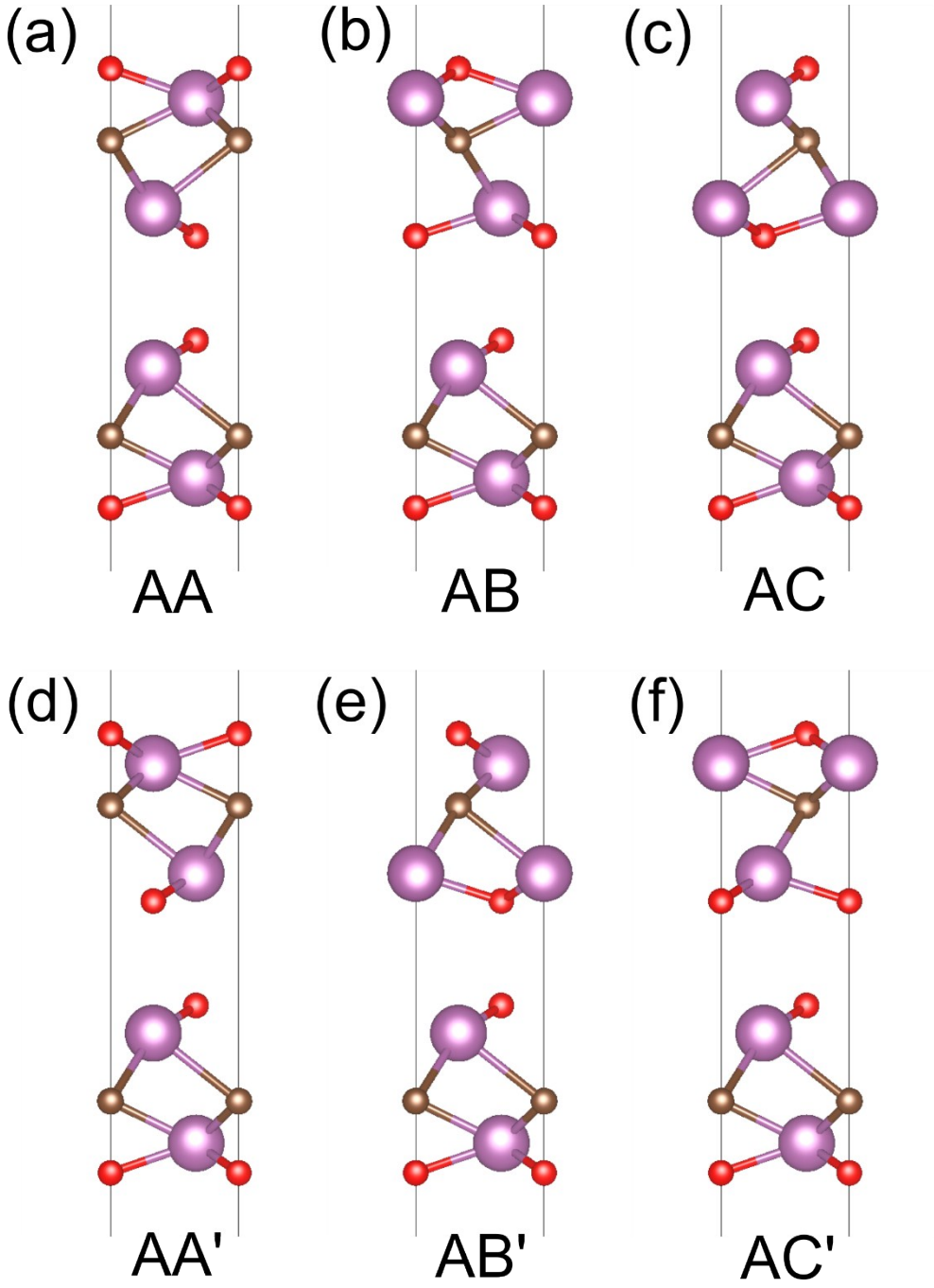

Figure S6. Different stacking configurations for bilayer UD Sc_2CO_2.

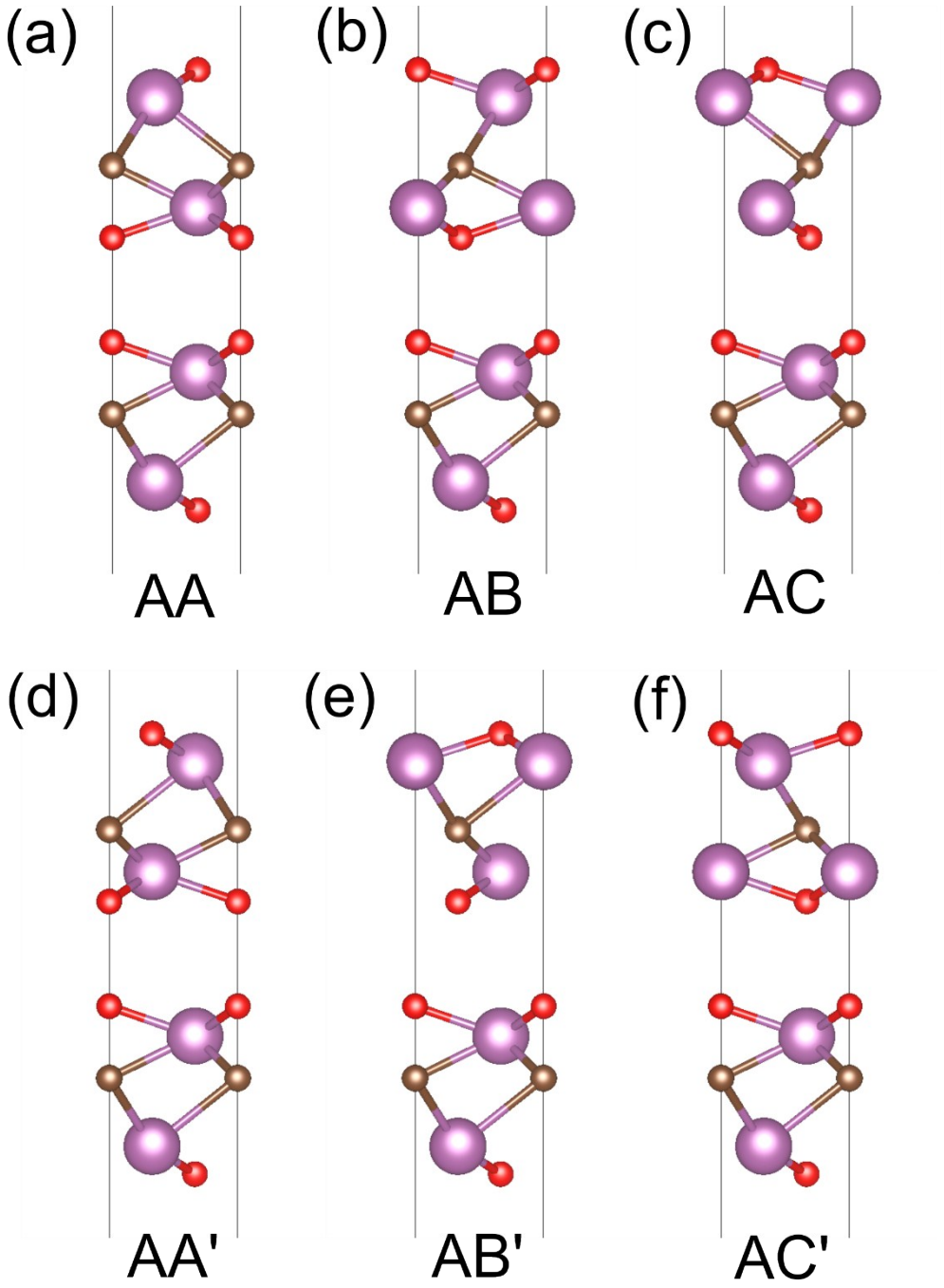

Figure S7. Different stacking configurations for bilayer DU Sc_2CO_2.

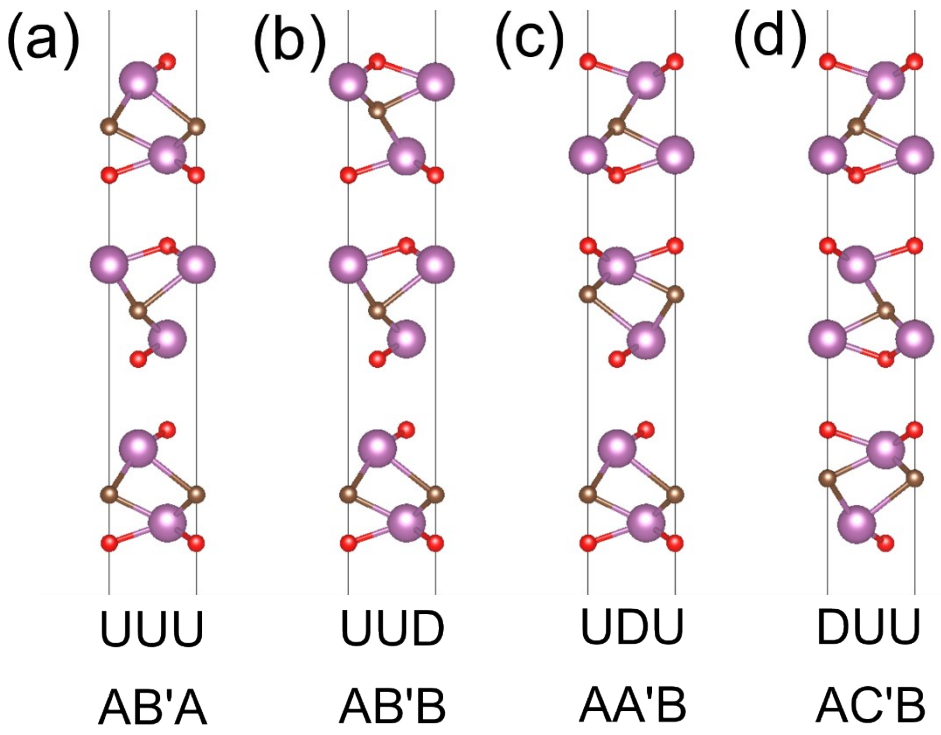

Figure S8. The stable stacking configurations for trilayers Sc_2CO_2.

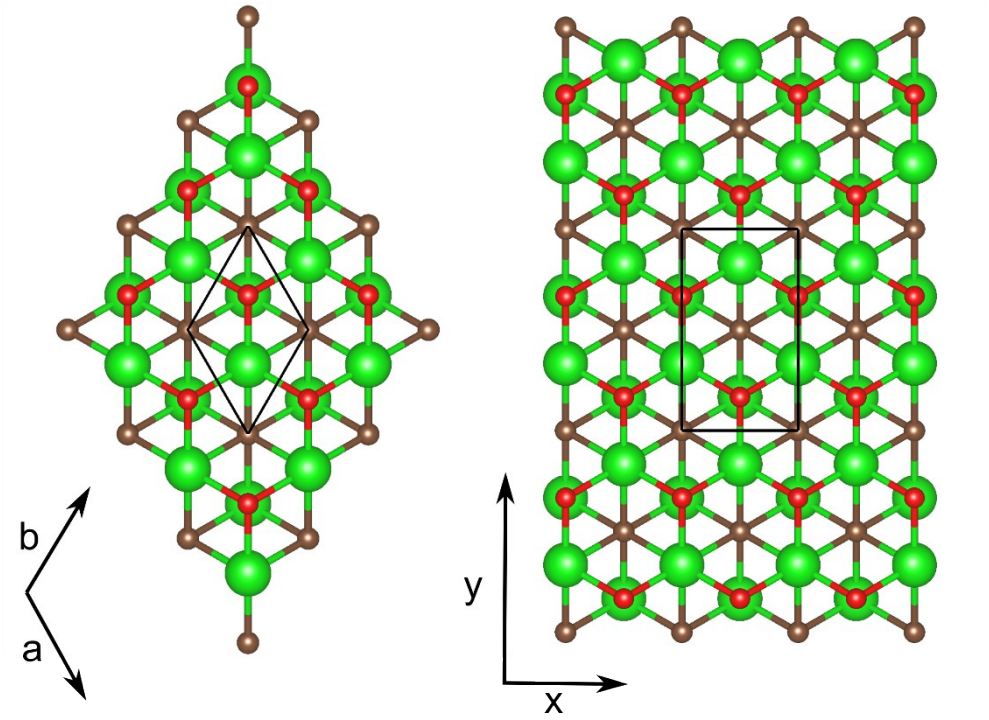

Figure S9. The hexagonal and orthogonal cells for multilayer MXene.

Table S1. The calculated total energy and lattice constant for four models of monolayer M_2CO_2 (M = Sc, Zr, Hf).

MXenes		a_0 (Å)	Energy (eV)
Zr_2CO_2	Model 1	3.590	-42.119
	Model 2	3.308	-48.640
	Model 3	3.275	-47.712
	Model 4	3.216	-46.550
Hf_2CO_2	Model 1	3.608	-45.867
	Model 2	3.271	-53.158
	Model 3	3.228	-52.155
	Model 4	3.163	-50.979
Sc_2CO_2	Model 1	3.429	-33.993
	Model 2	3.217	-41.212
	Model 3	3.406	-41.871
	Model 4	3.347	-41.737

Table S2. The calculated binding energy for different stacking configurations of bilayers and trilayers Zr_2CO_2.

Multilayers Zr_2CO_2		Binding energy (eV)
bilayers	AA	-0.417
	AB	-0.109
	AC	-0.170
	AA'	-0.105
	AB'	-0.265
	AC'	-0.265
trilayers	AAA	-0.844
	AAB	-0.531
	AAC	-0.593
	AAA'	-0.526
	AAB'	-0.689
	AAC'	-0.689

Table S3. The calculated binding energy for different stacking configurations of bilayers and trilayers Hf_2CO_2.

Multilayers Hf_2CO_2		Binding energy (eV)
bilayers	AA	-1.443
	AB	-0.498
	AC	-0.807
	AA'	-0.484
	AB'	-1.063
	AC'	-1.063
trilayers	AAA	-2.934
	AAB	-1.972
	AAC	-2.288
	AAA'	-1.959
	AAB'	-2.552
	AAC'	-2.549

Table S4. The calculated binding energy for different stacking configurations of bilayers Sc_2CO_2.

Bilayers Sc_2CO_2		Binding energy (eV)
UU	AA	-0.353
	AB	-0.268
	AC	-0.073
	AA'	-0.118
	AB'	-0.606
	AC'	-0.082
UD	AA	-0.059
	AB	-0.340
	AC	-0.340
	AA'	-0.841
	AB'	-0.066
	AC'	-0.108
DU	AA	-0.086
	AB	-0.275
	AC	-0.275
	AA'	-0.098
	AB'	-0.129
	AC'	-0.435

Table S5. The calculated binding energy for different stacking configurations of trilayers Sc_2CO_2.

Trilayers Sc_2CO_2		Binding energy (eV)
UUU	AB'A	-1.285
	AB'B	-0.777
	AB'C	-0.730
	AB'A'	-0.911
	AB'B'	-1.103
	AB'C'	-0.719
UUD	AB'A	-0.676
	AB'B	-1.458
	AB'C	-0.720
	AB'A'	-0.962
	AB'B'	-0.669
	AB'C'	-0.952
UDU	AA'A	-0.946
	AA'B	-1.287
	AA'C	-0.977
	AA'A'	-0.933
	AA'B'	-1.126
	AA'C'	-1.125
DUU	AC'A	-0.527
	AC'B	-1.052
	AC'C	-0.566
	AC'A'	-0.518
	AC'B'	-0.710
	AC'C'	-0.830

Table S6. The calculated binding energy for the most stable stacking configurations of tetra-layers Sc_2CO_2.

Tetra-layers Sc_2CO_2		Binding energy (eV)
UUUU	AB'AB'	-2.083
UUUD	AB'AA'	-2.143
UUDU	AB'BA'	-1.905
UDUU	AA'BC'	-1.904
DUUU	AC'BC'	-1.789
UUDD	AB'BC'	-2.077
UDDU	AA'CB'	-1.907
DDUU	AB'CA'	-1.669
UDUD	AA'BB'	-2.139
DUDU	AC'CB'	-1.733