

APPENDICES

APPENDIX A

THE CONFIGURATION AND PROPERTIES FOR 3D-TRANSITION METAL ATOMS DECORATED V_2CO_2

A.1 Optimization of different structures for V_2CO_2 surface

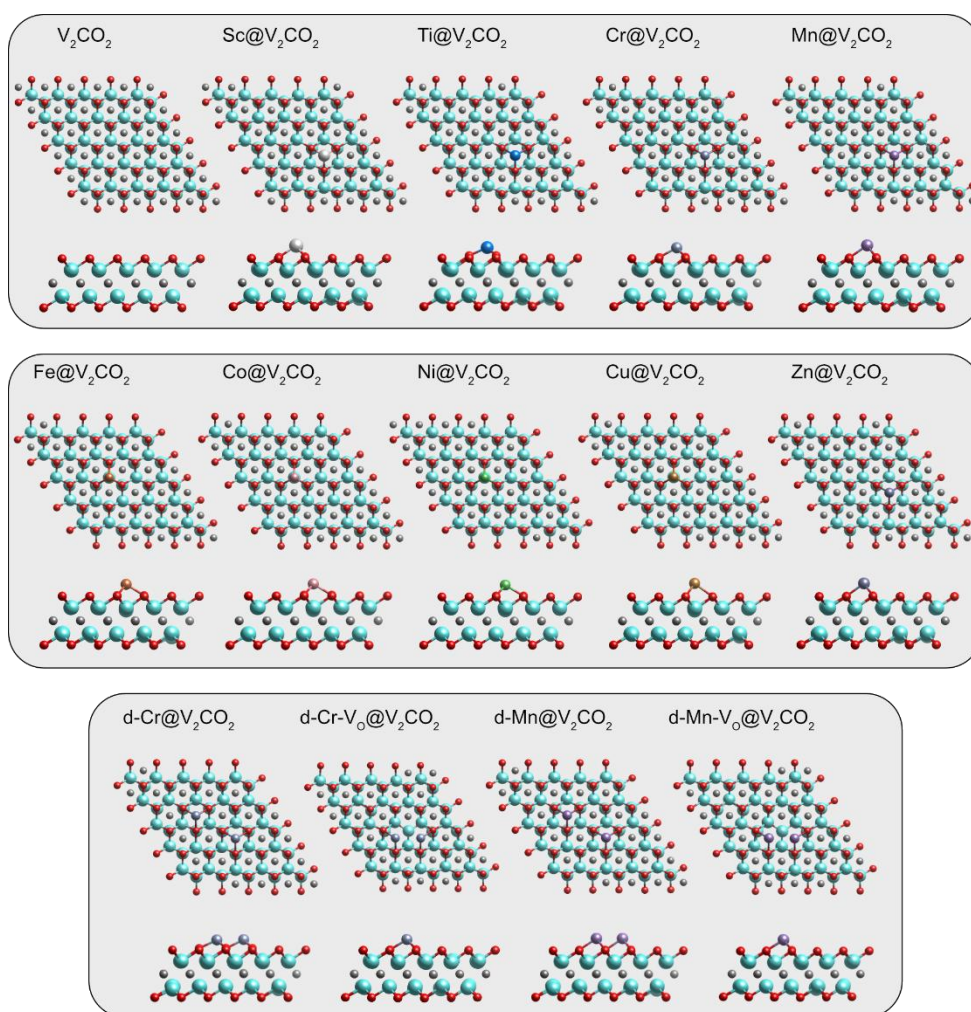


Figure A1 Optimized structures of the V_2CO_2 surface, $SA@V_2CO_2$ and $DA@V_2CO_2$.

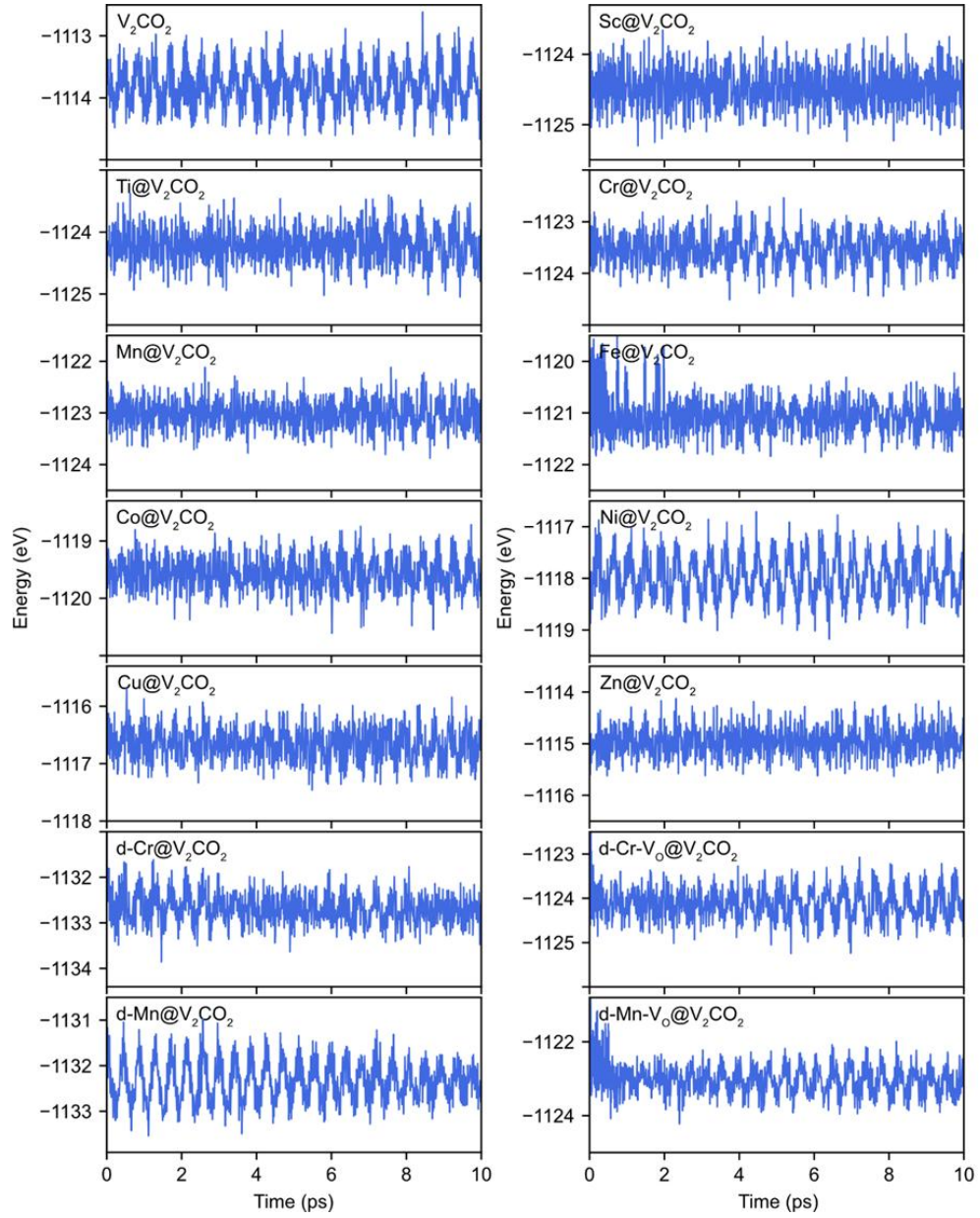


Figure A2 The fluctuation of total energy as a function of time along AIMD simulation at 300 K and corresponding initial and final configurations of bare, $SA@V_2CO_2$, and $DA@V_2CO_2$, a method used in similar a computational study (Singsen et al., 2022).

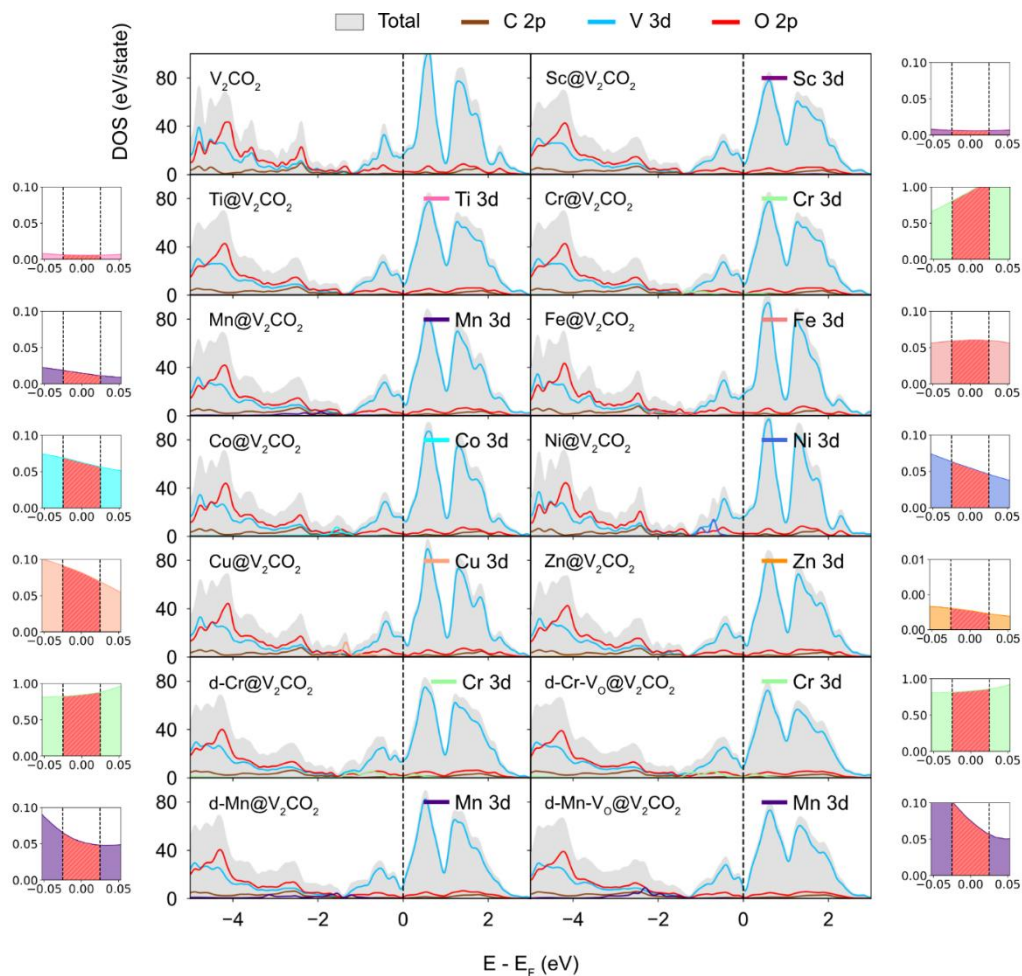


Figure A3 Projected Density of States (PDOS) for the bare, $\text{SA@V}_2\text{CO}_2$, and $\text{DA@V}_2\text{CO}_2$.

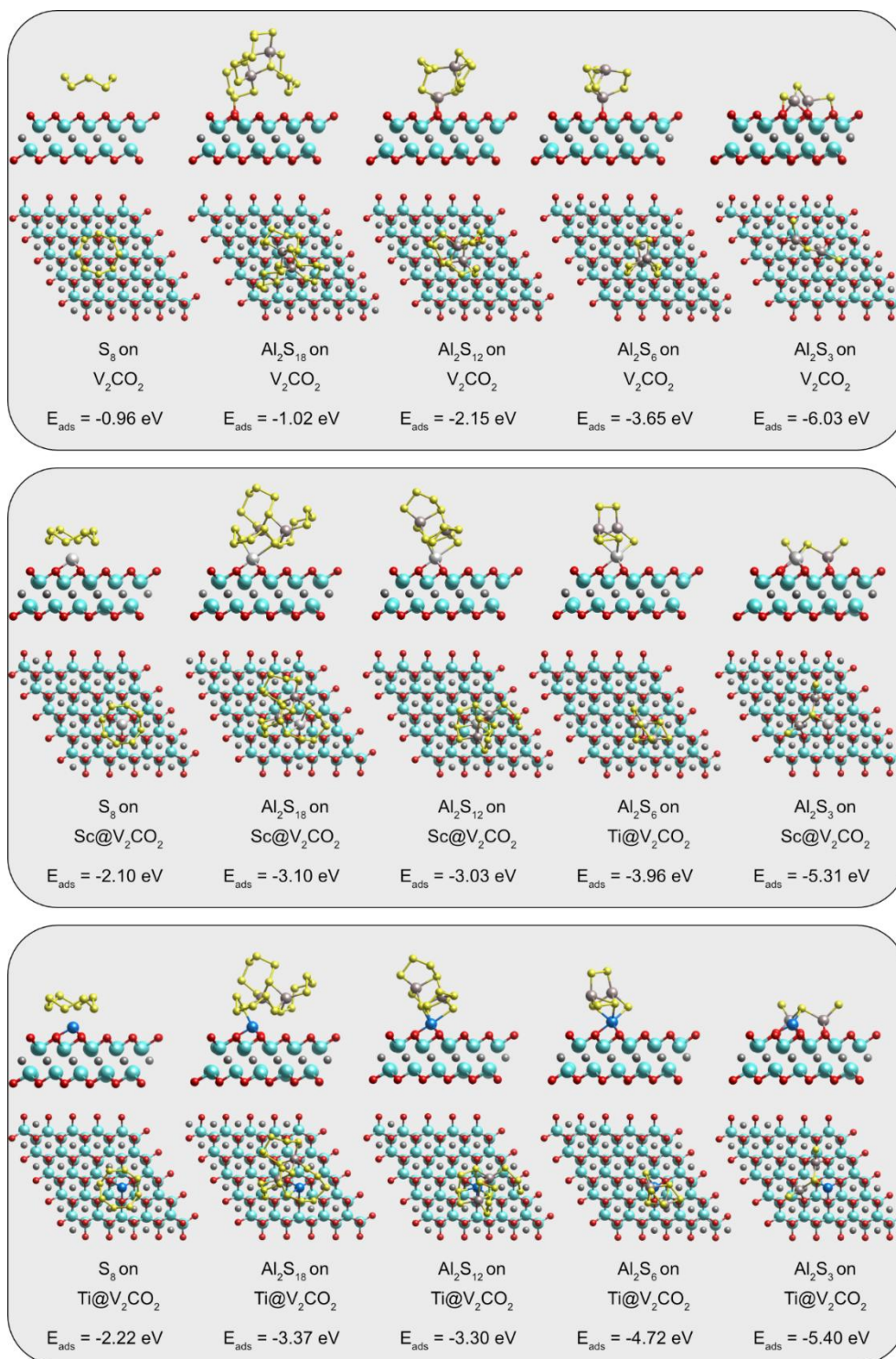


Figure A4 Optimized structures and adsorption energy of S_8 and Al_2S_n species on V_2CO_2 , $Sc@V_2CO_2$, and $Ti@V_2CO_2$.

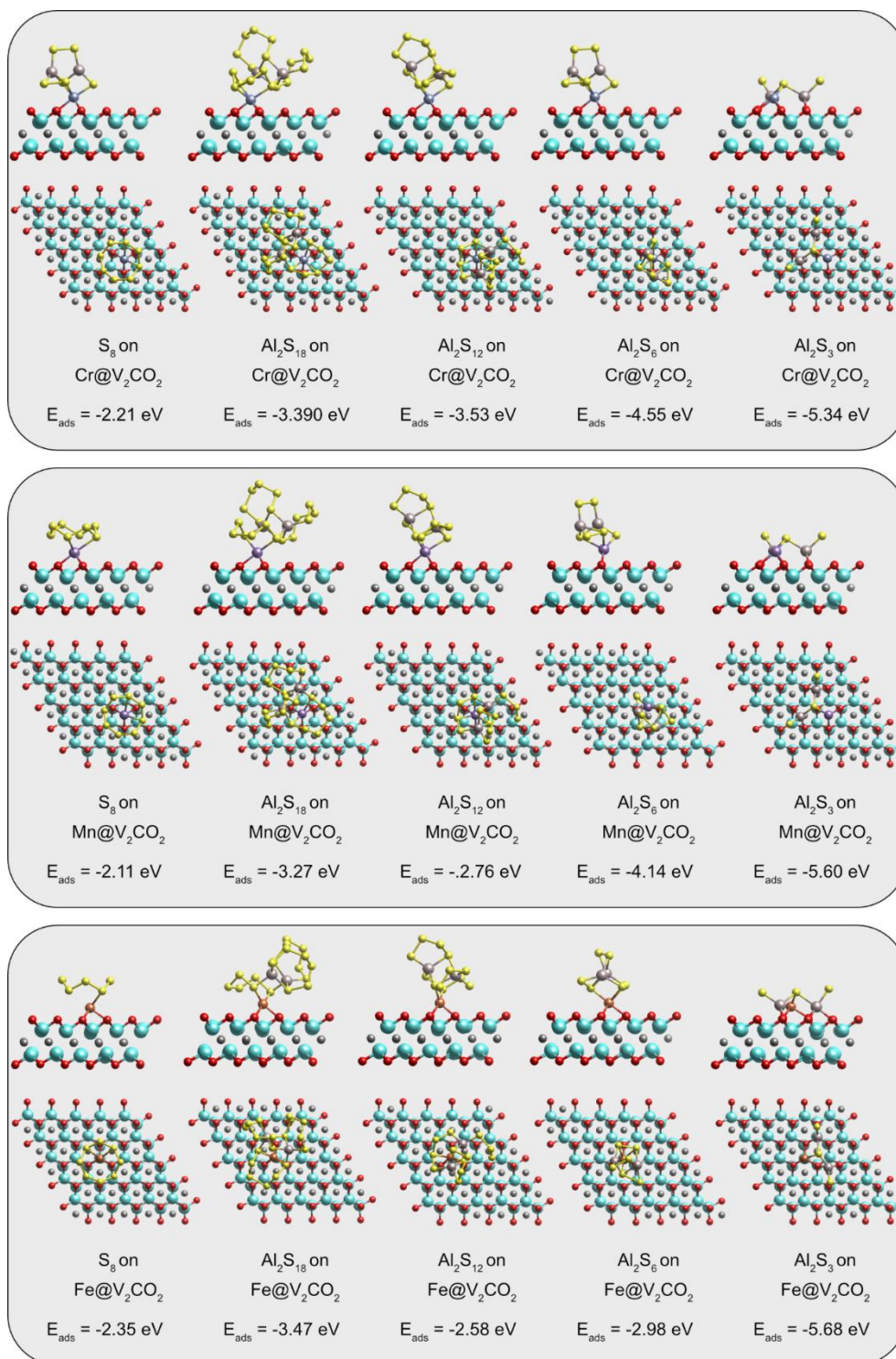


Figure A5 Optimized structures and adsorption energy of S_8 and Al_2S_n species on $\text{Cr@V}_2\text{CO}_2$, $\text{Mn@V}_2\text{CO}_2$, and $\text{Fe@V}_2\text{CO}_2$.

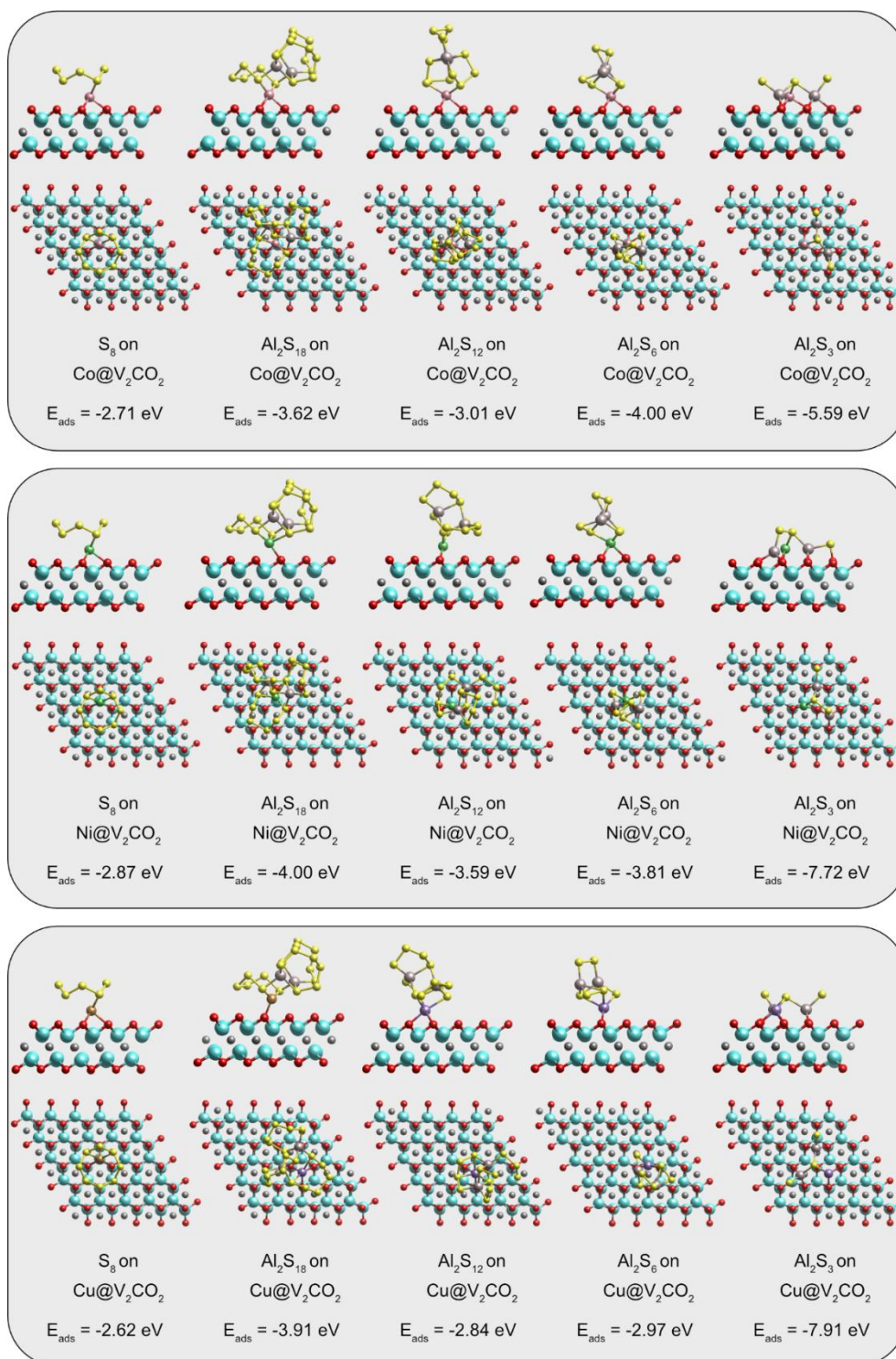


Figure A6 Optimized structures and adsorption energy of S₈ and Al₂S_n species on Co@V₂CO₂, Ni@V₂CO₂, and Cu@V₂CO₂.

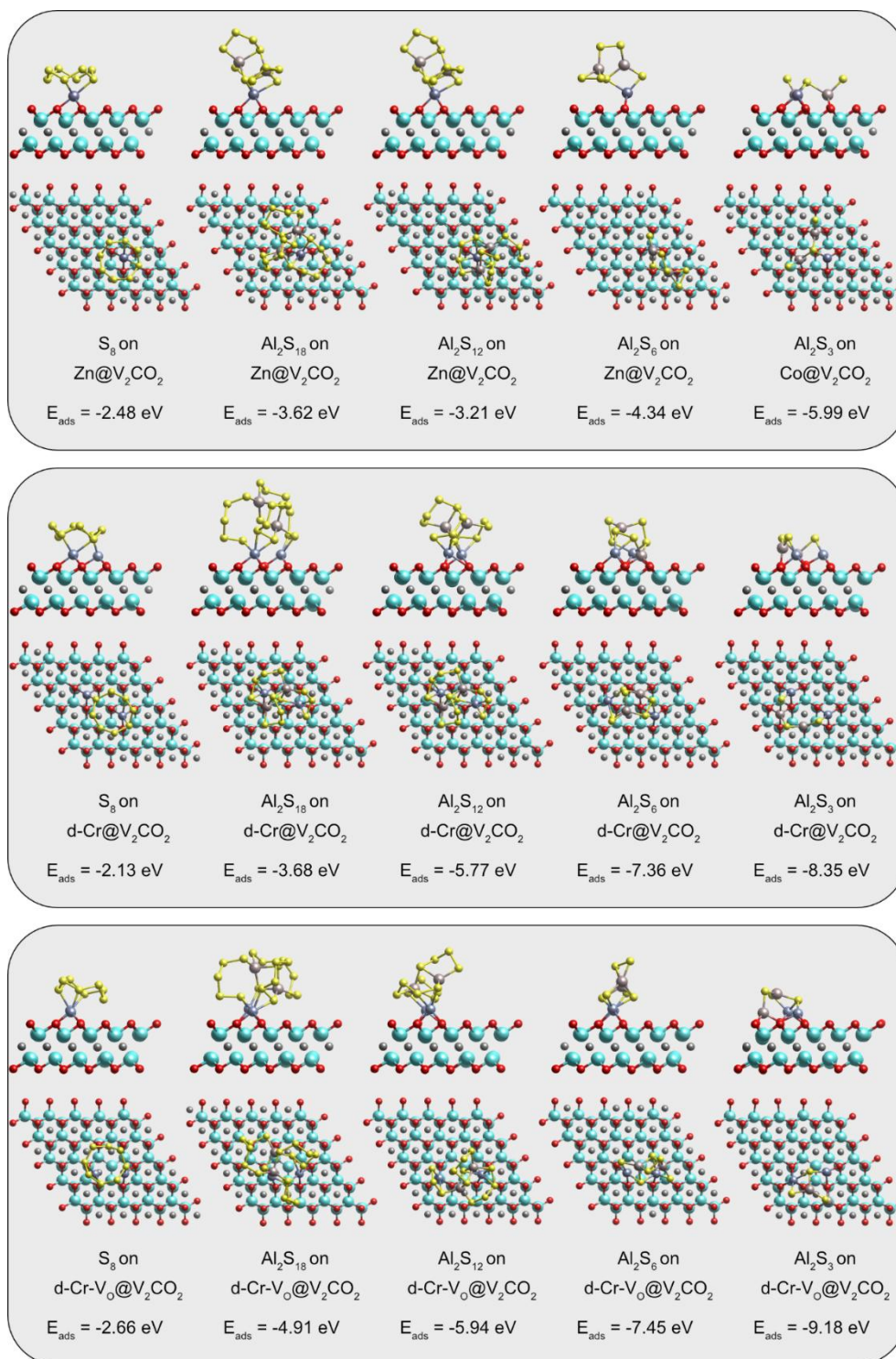


Figure A7 Optimized structures and adsorption energy of S_8 and Al_2S_n species on $Zn@V_2CO_2$, $d-Cr@V_2CO_2$, and $d-Cr-V@V_2CO_2$.

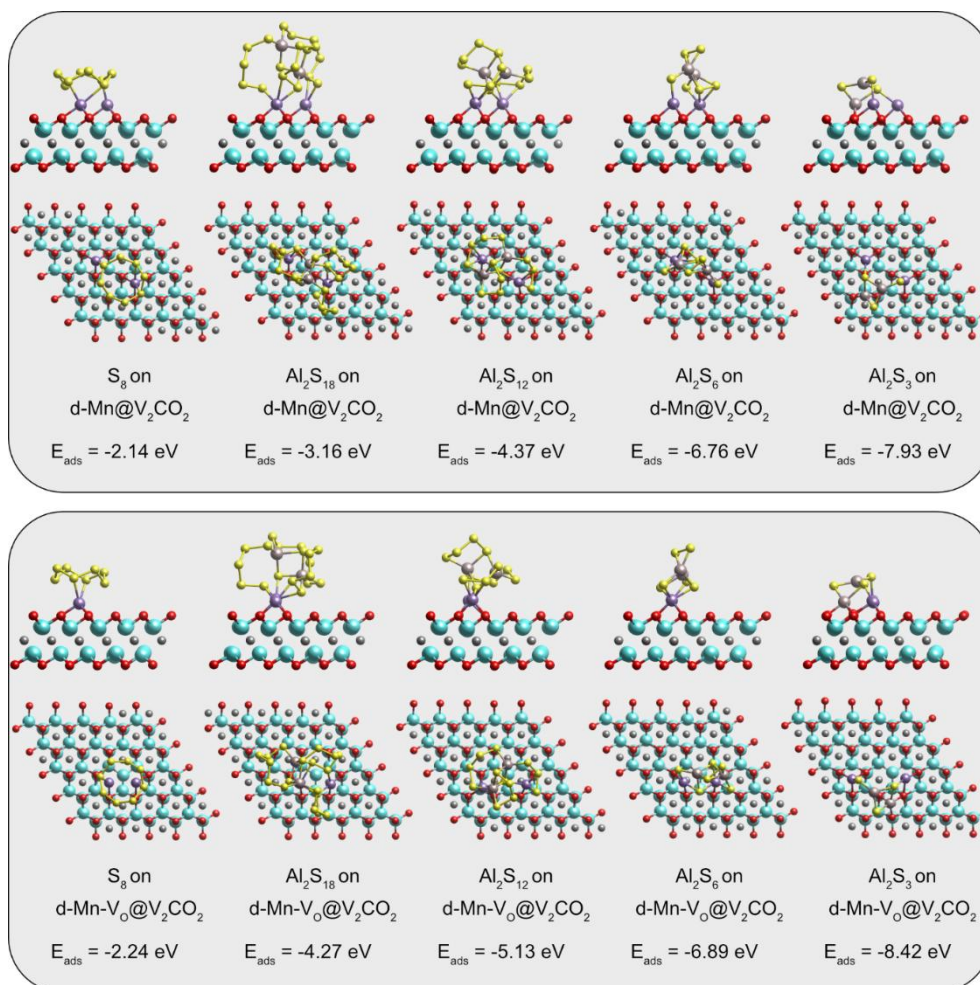


Figure A8 Optimized structures and adsorption energy of S_8 and Al_2S_n species on $\text{d-Mn@V}_2\text{CO}_2$, and $\text{d-Mn-V}_0\text{@V}_2\text{CO}_2$.

A.2 Sulfur reduction reactions and decomposition of Al_2S_3 for V_2CO_2 surface

Table A1 Gibbs free energy values for the reduction of S_8 and Al_2S_n species at $U = 0.83$ V (equilibrium potential).

Surfaces	S_8	$\text{Al}_2\text{S}_{18}^*$	$\text{Al}_2\text{S}_{12}^*$	Al_2S_6^*	Al_2S_3^*	Al_2S_3
Bare	0.00	1.37	-0.13	3.11	-2.35	0.00
Sc	0.00	-1.08	-1.21	4.17	6.03	0.00
Ti	0.00	-1.53	-2.38	1.78	-13.98	0.00
Cr	0.00	-2.16	-1.36	1.55	1.66	0.00
Mn	0.00	-1.67	-0.63	3.08	0.83	0.00
Fe	0.00	-1.88	-1.95	5.81	-0.10	0.00
Co	0.00	-2.12	-2.13	1.78	0.30	0.00
Ni	0.00	-2.62	-3.16	2.49	-16.28	0.00
Cu	0.00	-2.36	-1.73	5.91	-17.28	0.00
Zn	0.00	-2.07	-2.49	0.22	-3.22	0.00
d-Cr	0.00	-4.36	-9.89	-14.67	-26.71	0.00
d-Cr- V_O	0.00	-5.97	-10.37	-15.05	-32.21	0.00
d-Mn	0.00	-3.70	-7.26	-12.50	-21.93	0.00
d-Mn- V_O	0.00	-5.15	-8.79	-12.67	-26.12	0.00

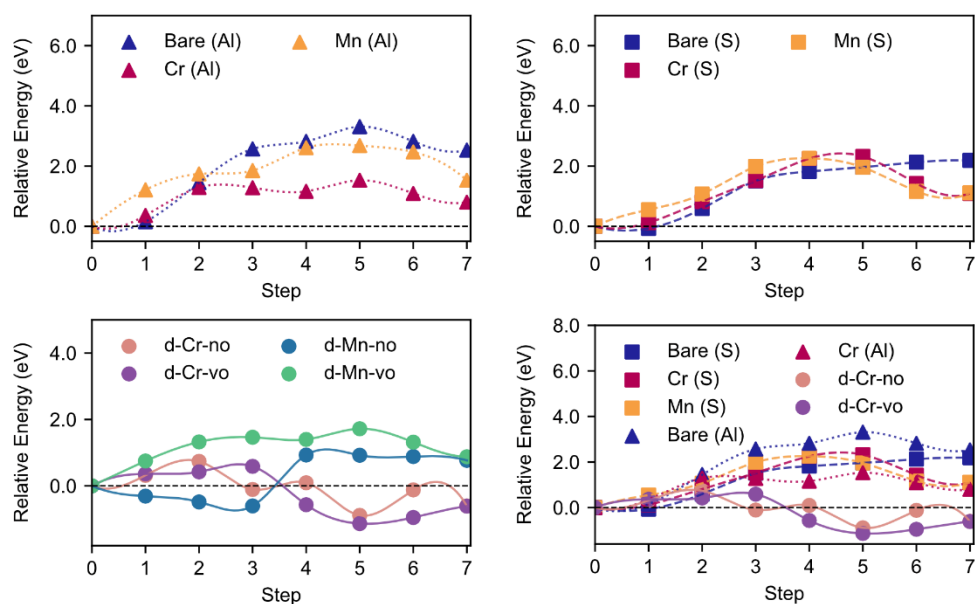


Figure A9 The decomposition of Al_2S_3 on bare, $\text{SA@V}_2\text{CO}_2$ including Cr, and Mn and $\text{DA@V}_2\text{CO}_2$ with and without V_O including Cr and Mn.

Reference

Singsen, S., Fongkaew, I., Hirunsit, P., & Suthirakun, S. (2022). Suppressing Polysulfides Shuttling and Promoting Sulfur Utilization via Transition Metal and Nitrogen Co-Doping on Graphdiyne Cathodes of Lithium-Sulfur Batteries: A First-Principles Modeling. *ACS Applied Energy Materials*, 5(8), 9722–9732.

APPENDIX B

PUBLICATION AND PRESENTATIONS

B.1 List of publication

Rattanaumpa, T., Panbo, P., Suthirakun, S., Kaewket, K., Wijitsak, J., Pinyou, P., and Ngamchuea, K. (2024). Catalysis of Oxygen Reduction Reaction by Iron Porphyrin and Its Sensing Application. J. Electroanal. Chem. 973: 118647.

B.2 List of presentation

Panbo, P., Kaewraung, W., K., Junkaew, A., and Suthirakun, S. (2024). First-Principles Study on the Performance of Single-Atom Supported V_2CO_2 as Cathode Materials of Aluminum-Sulfur Batteries. **The 27th International Annual Symposium on Computational Science and Engineering 2024 (ANSCSE27)**. 30 July - 3 August 2024, Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Thailand. (Oral presentation)