Electronic supplementary information (ESI)

Unexpected electro-catalytic activity of CO reduction reaction on Cr-embedded poly-phthalocyanine realized by strain engineering: A computational study

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Table S1. The DFT calculated total energy and strain energy of graphene and MoS_2 at specific strain (strain energy is obtained based on the relative energy without strain).

Strain	**Graphene**		**MoS_2**	
	0%	+20%	0%	+10%
Total Energy (eV)	-2072.77	-2069.48	-259791.62	-259790.07
Strain Energy (eV)	0	3.29	0	1.56

Table S2. The calculated limiting potential (U_L) values of CORR electro-catalysis with CH_4 as the product as reported in recent literatures.

Name	**U_L (V)**	**References**
MoS_2 with sulfur divacancies	-0.53	ChemSusChem, 2018[1]
$Fe_{19}@Cu_{60}$ CSNP	-0.58	Nanoscale, 2019[2]
W-anchored $Mo_2TiC_2O_{2-x}$	-0.20	Nanoscale, 2020[3]
B-doped BP under -7% strain	-0.38	J. Mater. Chem. A, 2020[4]
CrPPc under -5% biaxial strain	-0.09	This work

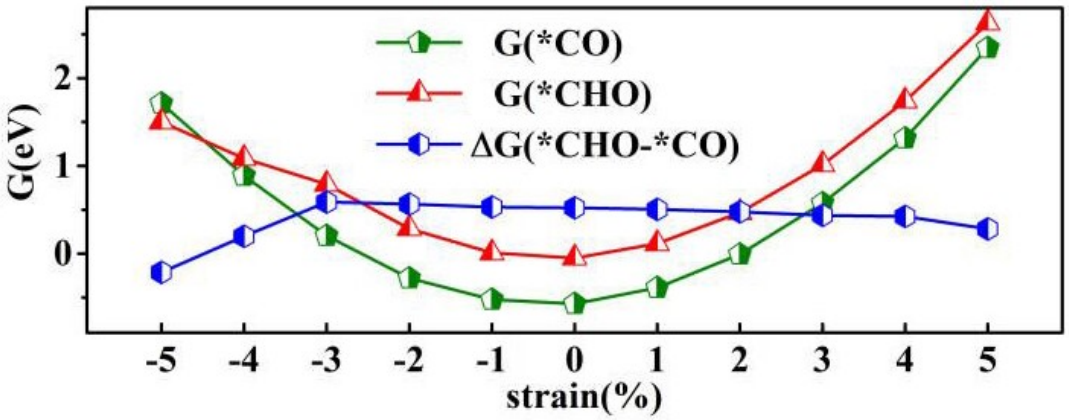

Figure S1. The free energy changes (ΔG) of *CO, *CHO and *CHO-*CO on CrPPc with biaxial strain of -5%~+5%.

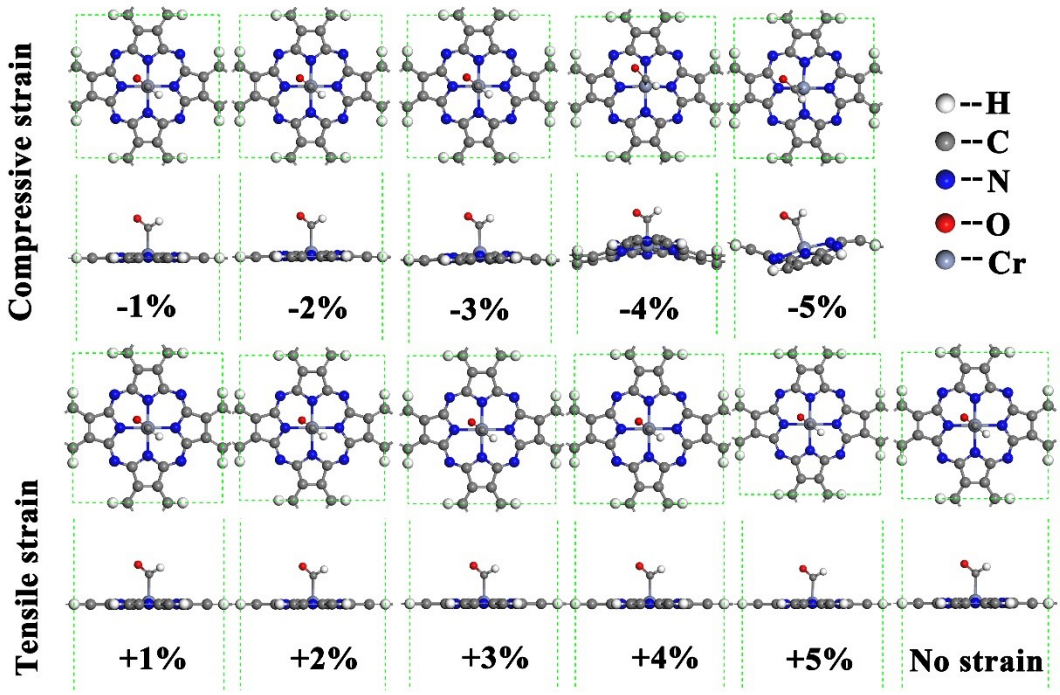

Figure S2. The optimized adsorption configurations of *CHO on CrPPc with biaxial strain of -5%~+5%.

References

1. Z. W. Chen, W. Gao, W. T. Zheng and Q. Jiang, *ChemSusChem*, 2018, **11**, 1455-1459.
2. H. Dong, C. Liu, Y. Li and D.-e. Jiang, *Nanoscale*, 2019, **11**, 11351-11359.
3. L. Li, B. Li, H. Guo, Y. Li, C. Sun, Z. Tian and L. Chen, *Nanoscale*, 2020, **12**, 15880-15887.
4. Z. Chen, X. Liu, J. Zhao, Y. Jiao and L. Yin, *J. Mater. Chem. A*, 2020, **8**, 11986-11995.