

# N-Doped CrS<sub>2</sub> Monolayer as a Highly-Efficient Catalyst for Oxygen Reduction Reaction: A Computational Study

Zengming Qin <sup>1</sup>, Zhongxu Wang <sup>1</sup>, Xiaofeng Li <sup>2</sup>, Qinghai Cai <sup>2</sup>, Fengyu Li <sup>3,\*</sup> and Jingxiang Zhao <sup>1,2,\*</sup>

<sup>1</sup> Key Laboratory for Photonic and Electronic Bandgap Materials, Ministry of Education, School of Physics and Electronic Engineering, Harbin Normal University, No. 1, Shida Street, Harbin 150025, China

<sup>2</sup> College of Chemistry and Chemical Engineering, Harbin Normal University, Harbin 150025, China

<sup>3</sup> School of Physical Science and Technology, Inner Mongolia University, Hohhot 010021, China

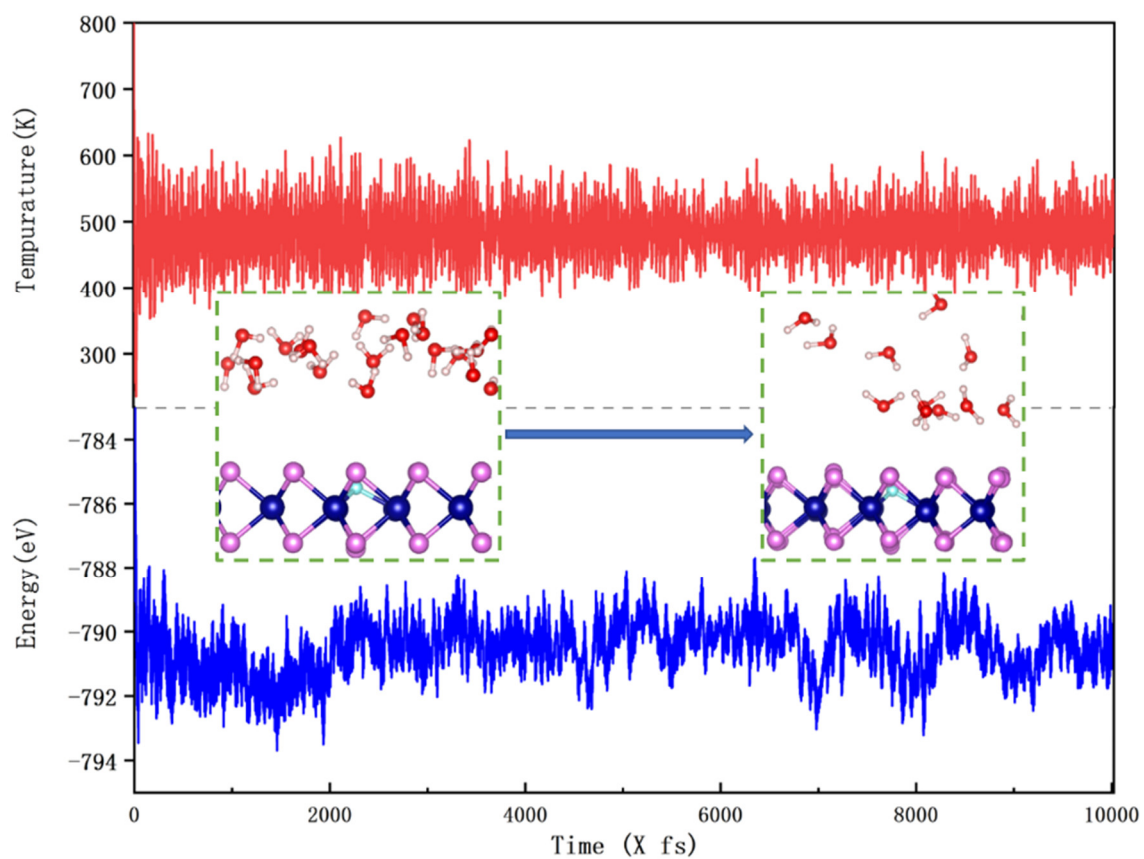
\* Correspondence: fengyuli@imu.edu.cn (F.L.); zhaojingxiang@hrbnu.edu.cn (J.Z.)

**Table S1.** The computed the overpotentials ( $\eta^{\text{ORR}}$ , V) at various energy cutoff (eV) or k-points.

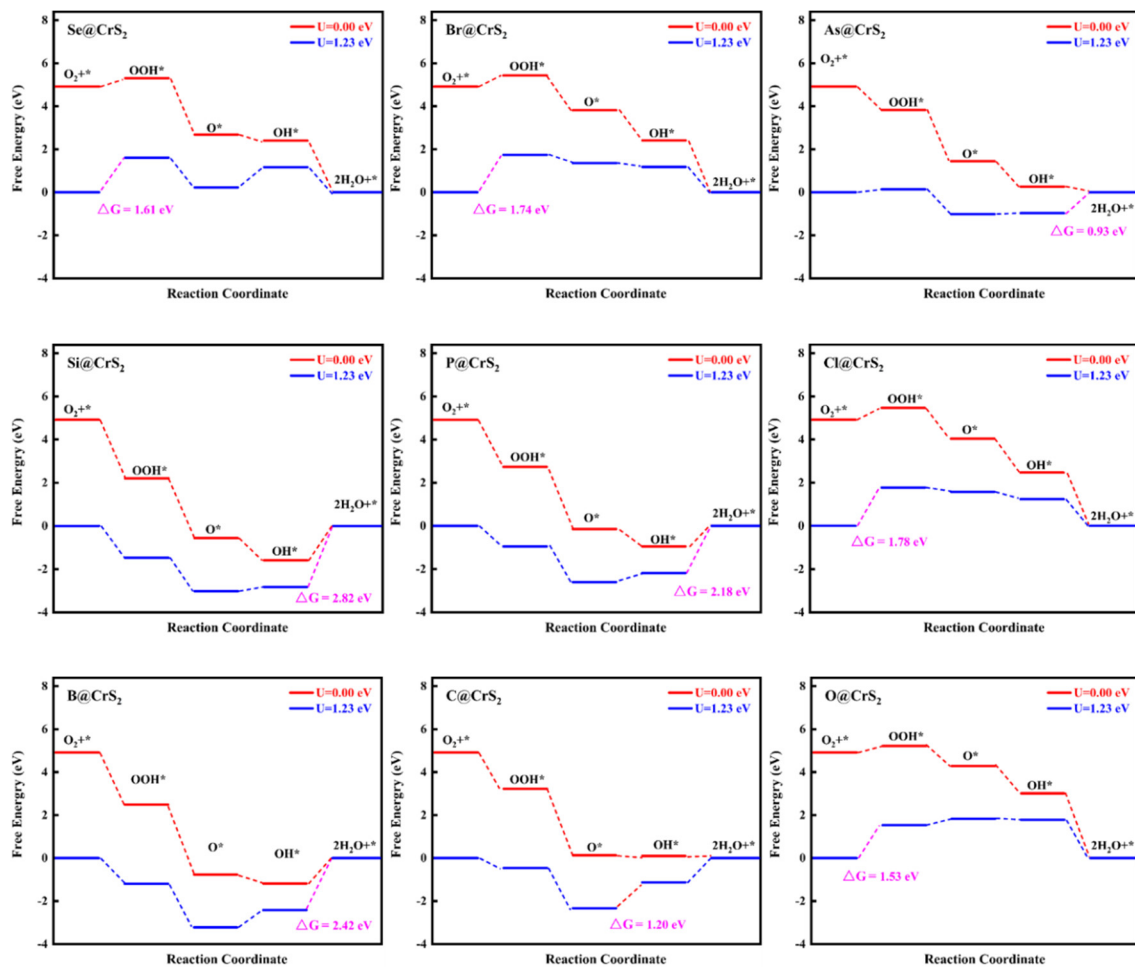
cutoff	$\eta^{\text{ORR}}$	k-point	$\eta^{\text{ORR}}$
400	0.43	$2 \times 2 \times 1$	0.40
450	0.44	$3 \times 3 \times 1$	0.41
500	0.41	$4 \times 4 \times 1$	0.41
500	0.41	$5 \times 5 \times 1$	0.41

**Table S2.** The computed the overpotential ( $\eta^{\text{ORR}}$ ) and the free adsorption energies ( $\Delta G$ , eV) for various X@CrS<sub>2</sub> materials.

	$\eta^{\text{ORR}}$	$\Delta G_{\text{O}^*}$	$\Delta G_{\text{OH}^*}$	$\Delta G_{\text{OOH}^*}$
pristine	1.78	0.00	0.55	4.08
B	2.42	-0.76	-1.19	2.49
C	1.20	0.13	0.10	3.23
N	0.41	1.65	0.82	4.07
O	1.53	4.29	3.01	5.22
Si	2.82	-0.56	-1.59	2.21
P	2.18	-0.14	-0.95	2.74
Cl	1.78	4.04	2.47	5.47
As	0.97	1.45	0.26	3.83
Se	1.61	2.68	2.40	5.30
Br	1.74	3.82	2.41	5.43



**Figure S1.** Total potential temperature and energy fluctuations after equilibration for N@CrS<sub>2</sub> in the AIMD simulation.



**Figure S2.** The computed free energy diagrams for ORR on different  $X@CrS_2$  systems.

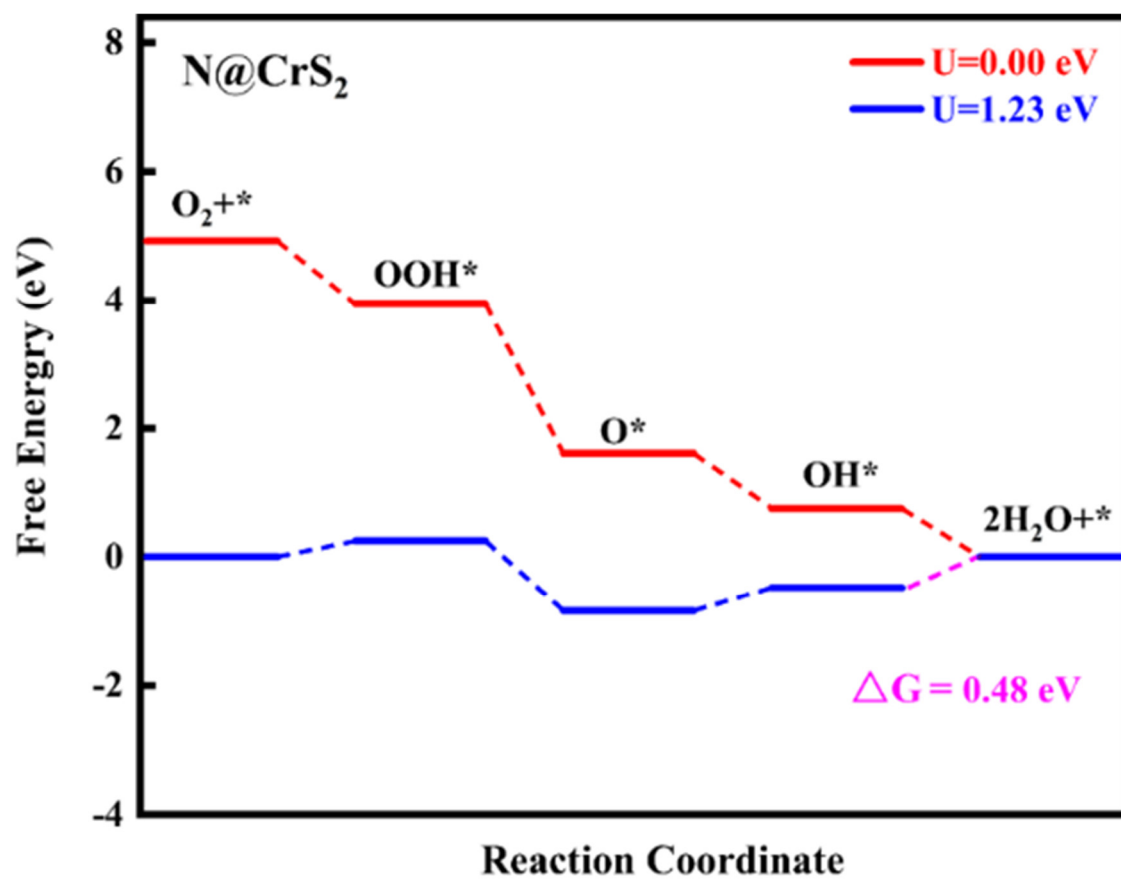
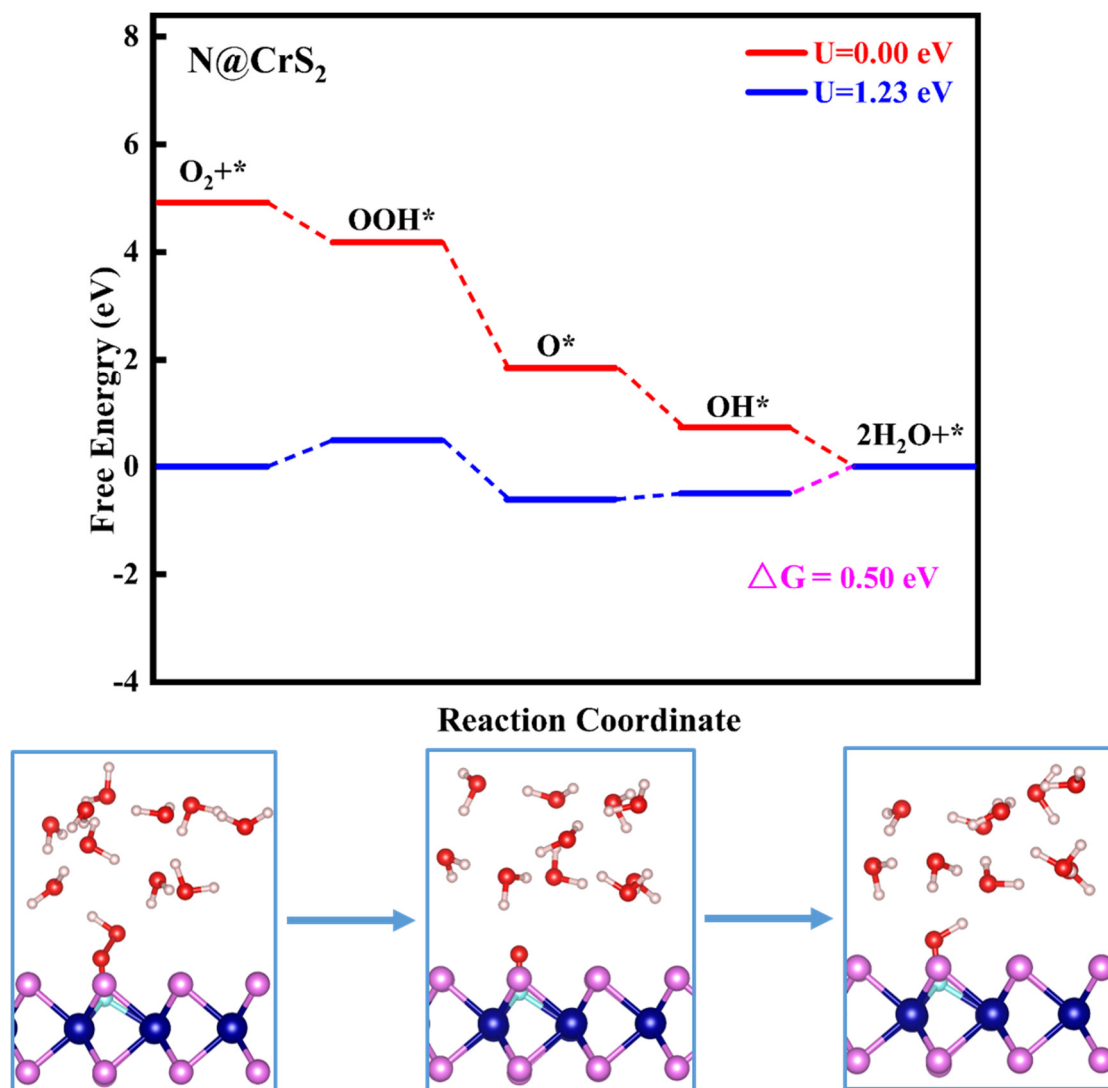


Figure S3. The computed free energy diagrams for ORR on N@CrS<sub>2</sub> with solvent effect.



**Figure S4.** The computed free energy diagrams and the corresponding intermediates configurations for ORR on N@CrS<sub>2</sub> with the explicit solvent models.