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

Supporting Information

Tuning catalytic activity of single Mo atom supported on graphene for nitrogen reduction via Se atom doping

Hong Yu Zhou, Jian Chen Li, Zi Wen*, Qing Jiang*

Key Laboratory of Automobile Materials, Ministry of Education, and School of Materials Science and Engineering, Jilin University, Changchun 130022, China

Table

Catalyst	ΔG_{RDS} (eV)	Refs.
MoN_2 monolayer	1.75	1
The flat surface of Sc, Y, Ti and Zr.	1.0~1.5	2
$Mo@N_3$	0.89	3
$Mo@C_4$	0.69	3
$Ti@N_4$	0.69	3
MoS_2	0.68	4
$Re@C_4$	0.60	3
MoC_6	0.54	5
Mo(110)	0.5	2
Fe doped MoN_2 monolayer	0.47	1
Mo/SeG	0.41	This work

Table S1. Calculated ΔG value of RDS for NRR on different systems.

Figures

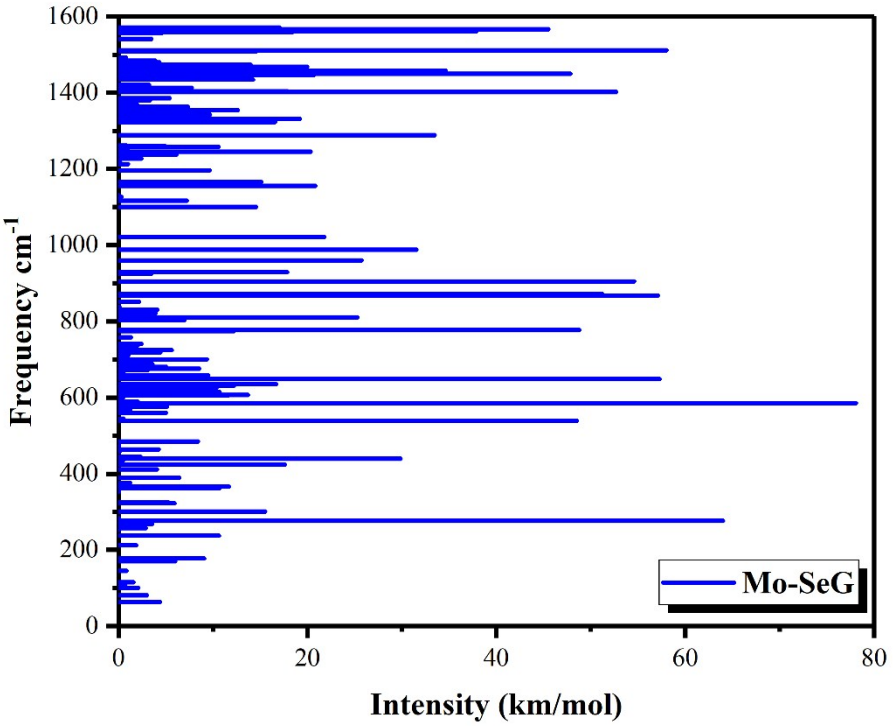

Figure S1. Frequency distribution of geometrically optimized Mo/SeG.

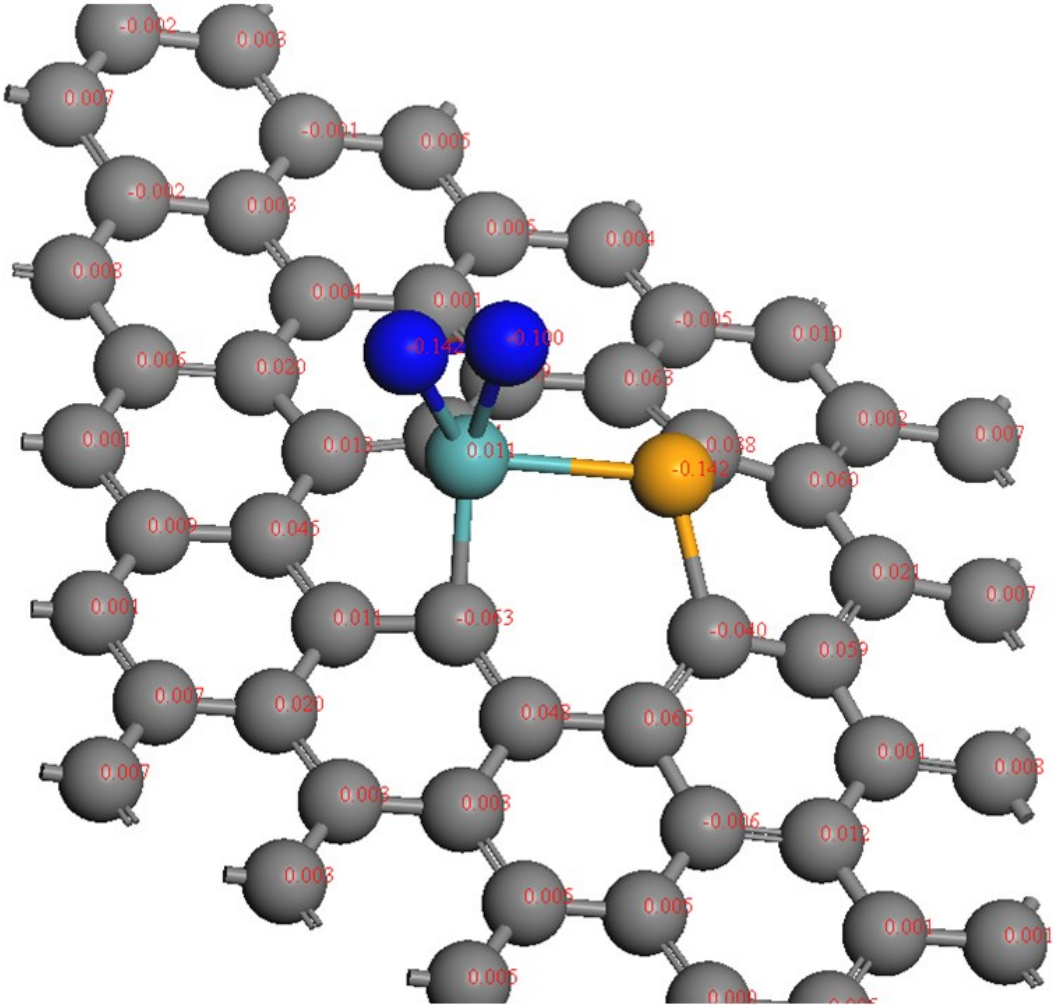

Figure S2. The mulliken charges distribution for Mo/SeG.

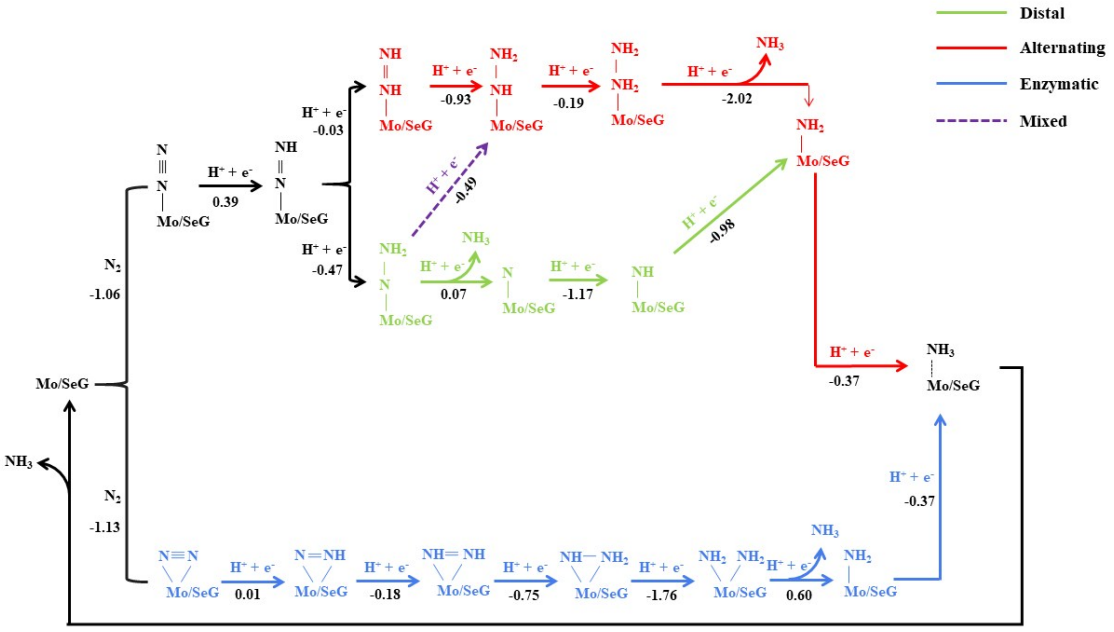

Figure S3. Schematic depiction of the possible mechanisms and the corresponding reaction energy (eV) for NRR by Mo/SeG; the dotted arrow represents the mixed mechanism that shuttle from distal to alternating mechanism.

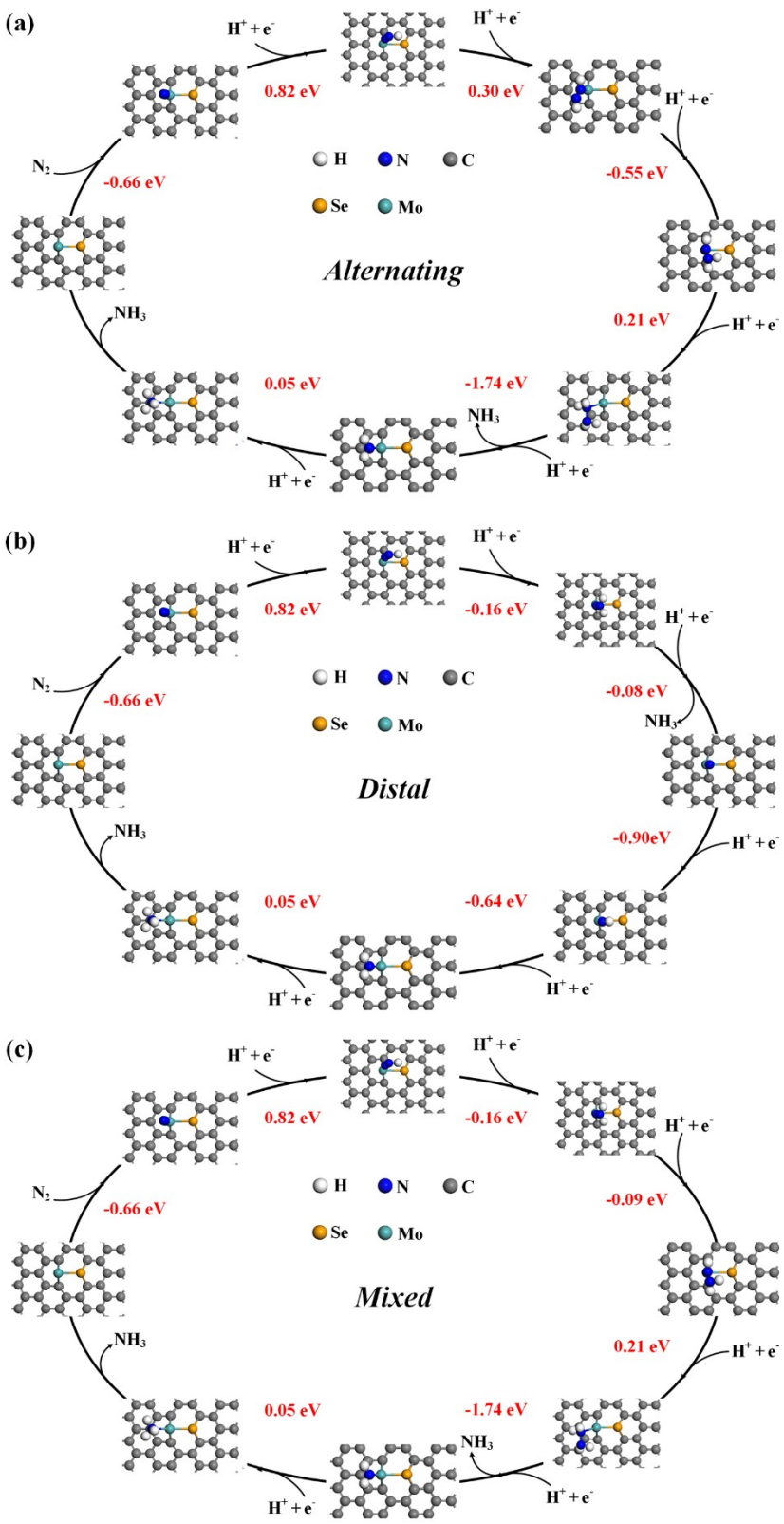

Figure S4. The optimized geometric structures of various intermediates along the reaction path of NRR proceed on Mo/SeG via (a) alternating, (b) distal and (c) mixed mechanism and the corresponding ΔG value.

References

1. Q. Li, L. He, C. Sun and X. Zhang, *J. Phys. Chem. C*, 2017, **121**, 27563-27568.
2. E. Skulason, T. Bligaard, S. Gudmundsdottir, F. Studt, J. Rossmeisl, F. Abild-Pedersen, T. Vegge, H. Jonsson and J. K. Norskov, *Phys. Chem. Chem. Phys.*, 2012, **14**, 1235-1245.
3. C. Choi, S. Back, N.-Y. Kim, J. Lim, Y.-H. Kim and Y. Jung, *ACS Catal.*, 2018, **8**, 7517-7525.
4. L. Zhang, X. Ji, X. Ren, Y. Ma, X. Shi, Z. Tian, A. M. Asiri, L. Chen, B. Tang and X. Sun, *Adv. Mater.*, 2018, **30**, 1800191.
5. Z. W. Chen, X. Y. Lang and Q. Jiang, *J. Mater. Chem. A*, 2018, **6**, 9623-9628.