

Synthesis of High Surface Area VS₂ for Nitrogen Reduction

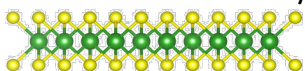
Logan M. Wilder, Taylor J. Aubry, Keenan Wyatt, Derek Vigil-Fowler, and Elisa M. Miller*

The National Renewable Energy Laboratory

Introduction

Transition Metal Dichalcogenides (TMDCs)

- Earth abundant
- High surface area 2D materials
- Tunable electrocatalysts

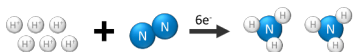


TMDC structure (S in yellow, M in green)

VS₂

- Metallic TMDC
- V edge-site predicted to be selective towards nitrogen reduction versus hydrogen evolution^{1,2}

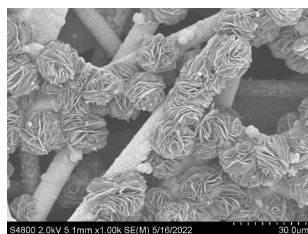
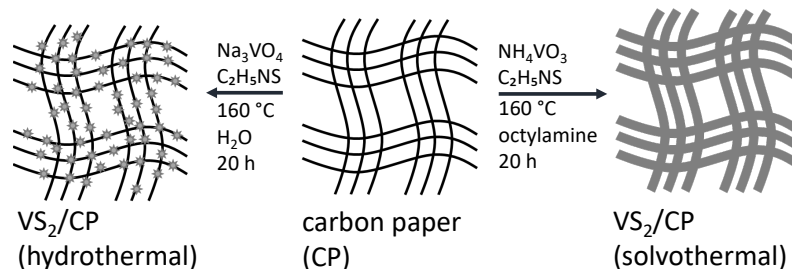
Electrochemical Nitrogen Reduction Reaction (NRR)



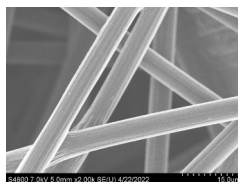
- Fossil-fuel free
- Generates NH₃ essential to agriculture

- 1) Li, F.; Chen, L.; Liu, H.; Wang, D.; Shi, C.; Pan, H. *The Journal of Physical Chemistry C* **2019**, *123* (36), 22221-22227.
- 2) Zhao, L.; Zhao, R.; Zhou, Y.; Wang, X.; Chi, X.; Xiong, Y.; Li, C.; Zhao, Y.; Wang, H.; Yang, Z.; Yan, Y.-M. *Journal of Materials Chemistry A* **2021**, *9* (44), 24985-24992.

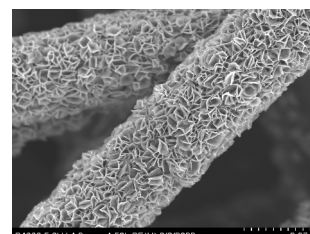
Hydrothermal Growth of Edge-Site Rich VS₂



VS₂/CP SEM image



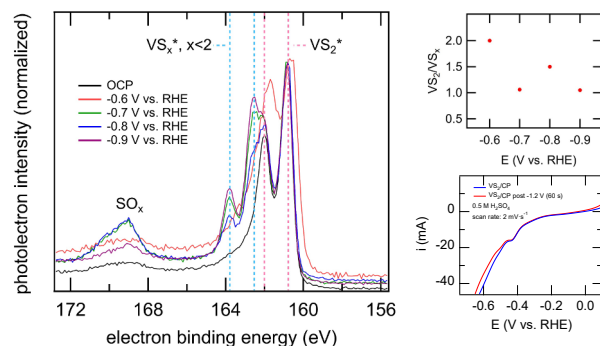
CP SEM image



VS₂/CP SEM image

VS₂/CP Electrochemical Generation of S Vacancies

Theory: S vacancy sites increase NRR activity



*VS₂ character indicated by peak position, XPS S:V ratio indicates VS₂

NRR Testing



reduce N₂ to NH₃ in H-cell

ex-situ quantification of NH₃

Material	NRR Activity?
Exfoliated TiS ₂	Negligible activity
Hydrothermal VS ₂ /CP	Negligible activity
Solvothermal VS ₂ /CP	Negligible activity
Electrochemical S vacancy (-0.9 V) VS ₂ /CP	Negligible activity

Future Work

- Introduce S vacancies to TMDC materials and observe effect on NRR activity
- TMDC electrocatalyst doping with transition metals
- TMDC nitrate reduction
- Photoelectrochemical NRR with VS₂ and MoS₂ electrodes



Source: Energy Environ. Sci., 2021, 14, 6242



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