

Review of: "Ti2N nitride MXene evokes the Mars-van Krevelen mechanism to achieve high selectivity for nitrogen reduction reaction"

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Potential competing interests: The author(s) declared that no potential competing interests exist.

Reviewer: The author presented a two-dimensional (2D) Ti2N nitride MXene as an efficient electrocatalyst for the N2 reduction reaction at room temperature and atmospheric in 0.1 M HCl. Although the authors believe the Mar van Krevelen(MvK) mechanism solves the low selectivity problem encountered by the electrochemical nitrogen reduction reaction to ammonia, the performance is not impressive in terms of the NH3 yield rate. How to concurrently obtain high NRR activity and FE is critically important. Another concern is that the contribution of N in the catalyst to the NRR performance is not well established. The presentation and clarification need to be significantly improved before further consideration. Other suggestions to the authors:

- 1. The authors emphasize that the MvK mechanism improves the selectivity of NRR without further theoretical evidence for its existence.
- 2. In the Figure 2d, the current densities of N2-saturated and Ar-saturated are same at -0.25 V, however, the paper have significant difference catalytic performance under two conditions at -0.25 V. Maybe the ammonia is not from nitrogen reduction.
- 3. According to Figure 3 listed by the author, it can be concluded that the NH3 production rate of Ti2N in the Ar saturated electrolyte cannot be ignored. Please give further explanation.
- 4. Has the author tested the performance of the catalyst in other solutions, such as sulfuric acid, sodium sulfate and other solutions?
- 5. The authors should provide long-term durability test data to prove the electrocatalytic stability of the catalyst.
- 6. The detection of NH4+ is extremely sensitive, but there is only one method in this paper. The author should provide the result of lon chromatography detection or N15 isotope detection.
- 7. The author should provide comparison with similar transitionmetal catalysts to prove that the FE of Ti2N is the highest.
- 8. How did authors treat Ar and N2 gases prior to experiments? It is not recommended to use them as purchased because the trace impurities exist in them can contribute to misleading NRR.
- 9. The authors argue that two-dimensional materials have a higher specific surface area, have you measured it?



10. how can you guarantee the yield and purity of the catalyst?