

## A $\text{Ti}_3\text{C}_2\text{O}_2$ Supported Single Atom, Trifunctional Catalyst for Electrochemical Reactions

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**Abstract :** Water splitting and rechargeable air-based batteries are emerging as new renewable energy storage and conversion technologies. However, the discovery of suitable catalysts with high activity and low cost remains a great challenge. In this work, we report a single-atom trifunctional catalyst, namely  $\text{Ti}_3\text{C}_2\text{O}_2$  supported single Pd atom ( $\text{Pd}_1@ \text{Ti}_3\text{C}_2\text{O}_2$ ), for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). This catalyst is selected from 12 candidates and possesses low overpotentials of 0.22 V, 0.31 V and 0.34 V for the HER, OER and ORR, respectively, making it an excellent electrocatalyst for both overall water splitting and rechargeable air-based batteries. The superior OER and ORR performance originates from the optimal d band center of the supported Pd atom. Moreover, the excellent activity can be maintained even if the single Pd atoms aggregate into small clusters. This work offers new opportunities for advancing the renewable energy storage and conversion technologies and paves a new way for the development of multifunctional electrocatalysts.

**Keywords :** DFT, SACs, OER, ORR, HER

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