2D Layered MPX_3 Performance for Water Splitting Reactions

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Two-dimensional (2D) layered materials are currently one of the most explored materials for developing efficient and stable electrocatalysts for energy conversion applications. Some of the 2D metal phosphorous trichalcogenides, $M_2P_2X_6$ or simply MPX_3, have been reported to be useful catalysts for water splitting,[1] although the results have been less promising for the sluggish oxygen evolution reaction (OER) due to insufficient activity or compromised stability.

We report on the water splitting performance of a series of MPX_3 (M^{2+} = Mn, Fe, Co, Zn, Cd; X = S, Se). For the series of MPX_3, $CoPS_3$ yields the best results with an overpotential within the range of values usually obtained for IrO_2 or RuO_2 catalysts. The liquid-phase exfoliation of $CoPS_3$ improves the OER activity due to the abundant active edges of the downsized sheets, accompanied by the presence of surface oxides. The influence of the OER medium and the underlying substrate electrode is studied, with the exfoliated $CoPS_3$ reaching the lowest overpotential also able to sustain high current densities, with excellent stability after multiple cycles or long-term operation.

The photoelectrochemical (PEC) responsivity of MPX_3 was also tested in the OER region, with excitation wavelengths from 385 to 700 nm, is reported. [3] The experimentally determined optical bandgaps of the MPX_3 materials range from 1.5 eV for $FePSe_3$ to 3.7 eV for $ZnPS_3$. At +1.23 V vs. RHE, the PEC activity in the OER region of $MnPSe_3$ exhibits superior performance, while the exfoliation of $CoPS_3$ improves its PEC activity up to double in contrast with its bulk counterpart. The influence of the substrate and applied potential is also optimized.

References

[1] R. Gusmão et al., Angew. Chemie Int. Ed. 58 (2019) 9326–9337.
[2] F.M. Oliveira et al. ACS Appl. Mater. Interfaces. 13 (2021) 23638–23646.
[3] F.M. Oliveira et al., Adv. Mater. Interfaces. (2021) 2100294.

Figures

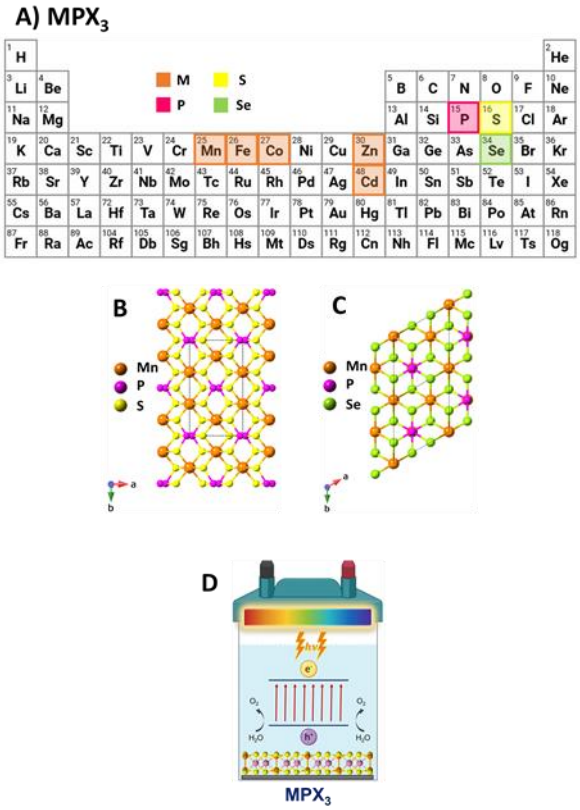

Figure 1: (A) Periodic table in which the filled blocks represent the elements selected for the synthesis of MPX3 materials. Top (c-axis) view of the crystal structures of (B) MnPS3 and (C) MPSe3. Color scheme: Mn – orange, P – pink, S – yellow, Se – green. D) Scheme of the photoelectrochemical response of MPX3 for OER.