# Article information:

Activating Basal Planes of NiPS3 for Hydrogen Evolution by Nonmetal Heteroatom Doping - Wang - 2020 - Advanced Functional Materials - Wiley Online Library
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# Article summary:

1. Nonmetal heteroatom doping can improve the hydrogen evolution reaction (HER) activity of NiPS3 by transforming its semiconducting nature and activating surface sites for hydrogen adsorption.

2. B and C atoms are favorable for replacing P in NiPS3, while N and O tend to replace S.

3. The electronic structure of dopants plays a crucial role in HER activity enhancement, with B- and especially, C-doped NiPS3 exhibiting the optimum HER performance among all single nonmetal-doping samples.

# Article rating:

Appears moderately imbalanced: The article provides some useful information, but is missing several important points or pieces of evidence that would be required to present the discussed topics in a balanced and reliable way. You are encouraged to seek a more balanced perspective on the presented issues by exploring the provided research topics and looking at different information sources.

# Article analysis:

The article discusses the development of a new class of electrocatalysts for hydrogen evolution reaction (HER) using nonmetal heteroatom doping in metal trichalcogenidophosphates (MTPs). The authors highlight the importance of finding an electrocatalyst that is low cost, stable, and highly active for HER. They note that while noble metal catalysts like Pt-based catalysts are highly efficient, their scarcity and high cost limit their practical applications. Non-noble-metal-based materials like transition metal chalcogenides and phosphides have attracted attention due to their abundance and relatively high electrocatalytic performance.

The authors focus on NiPS3 as a potential electrocatalyst for HER but note that its activity is far inferior to many other phosphosulphides despite having abundant PSx functional groups. Theoretical calculations reveal that only undercoordinated edge atoms in NiPS3 participate as active sites while the sites on its basal plane remain inert due to the intrinsic semiconducting nature of NiPS3, which also leads to slow electron transfer along the basal plane.

To improve HER activity, the authors introduce nonmetal heteroatom doping into NiPS3 and demonstrate that B- and C-doping can transform the semiconducting NiPS3 to a meal and greatly activate surface sites for hydrogen adsorption on NiPS3 catalyst leading to optimal HER activity. They establish an interplay between hydrogen adsorption free energy and p-band center of active sites and correlate directly HER activity of doped NiPS3 with electronic structures of dopants.

While the article provides valuable insights into developing new electrocatalysts for HER using nonmetal heteroatom doping in MTPs, it may have some biases. For example, it focuses solely on the benefits of nonmetal heteroatom doping without exploring any potential risks or drawbacks associated with this approach. Additionally, it does not present any counterarguments or alternative approaches to developing electrocatalysts for HER. The article also appears to be promotional in nature, highlighting the potential of MTPs as a new class of electrocatalysts without discussing any limitations or challenges associated with their development and implementation.

Overall, the article provides valuable insights into developing new electrocatalysts for HER using nonmetal heteroatom doping in MTPs. However, it may have some biases and limitations that should be considered when interpreting its findings.

# Topics for further research:

* Limitations of nonmetal heteroatom doping in electrocatalysts for HER
* Alternative approaches to developing electrocatalysts for HER
* Challenges associated with implementing MTPs as electrocatalysts
* Comparison of noble metal and non-noble metal electrocatalysts for HER
* Role of surface area and morphology in electrocatalytic activity for HER
* Strategies for improving electron transfer in semiconducting electrocatalysts for HER

# Report location:

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