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Data mining in photocatalytic water splitting over perovskites literature for higher hydrogen production

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GRAPHICAL ABSTRACT



Highlights

- Photocatalytic water splitting (PWS) over perovskites literature were analyzed.
- Database containing 540 instances from 151 publications on PWS was constructed.
- Data were modeled by association rule mining, decision tree & random forest.
- Past trends were determined, effective materials and methods were identified.
- Heuristics and models for high hydrogen production rates were developed.

Abstract

A database containing 540 cases from 151 published papers on photocatalytic water splitting over perovskites was constructed and analyzed using data mining tools; the factors leading high hydrogen production were identified by association rule mining while some useful heuristics for the future studies were developed by decision tree analysis. Additionally, the predictive models were developed using random forest regression.

In about half of the works, the perovskites were doped by A-site, B-site or both; however, only some portion of doped catalysts had better activity than plain perovskites while doping also improved stability in some cases. The effect of co-catalyst on activity seems to be also irregular; no definitive conclusion could be drawn. The effects of preparation methods on surface area, band gap and crystal

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