Machine Learning Guided and Accelerated Development of Semiconductor Photothermal Materials Using Doping Strategy to Modify Bandgap for Enhancing Solar Water Evaporation

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Solar water evaporation (SWE) outstands as a promising method to solve the global freshwater shortage due to its lower cost, green and sustainable. Semiconductors photothermal materials (SPMs), with modifiable bandgap, and high performance, exhibiting excellent prospects for practical SWE. However, the precise influence of SPMs properties on evaporation performance remains unclear, necessitating long time and large costs to develop by trial-and-error tests. Machine learning (ML) emerges as a data-driven approach to achieve feature classification and performance prediction in evaluating SPMs. In this project, four ML models were employed to analyze the database collected from the latest research articles of SPMs, to achieve features classification (BG, A, TC, IL/sun, T, H) and evaporation performance prediction. Shapley Additive Explanation analysis revealed the impact features for evaporation performance of SPMs. Moreover, experimental validation for the ML model's reliability was achieved doping sodium borohydride (NaBH4) to titanium dioxide (TiO2) for narrowing bandgap by calcining under 300 °C, 500°C and 700 °C for one hour, respectively. Various characterizations were analyzed through SEM, XPS and UV-Vis confirmed Ti4+ converted into Ti3+, resulting in forming oxygen vacancy to narrow bandgap of four samples from 3.36 eV (P25), 3.33 eV (300°C), 3.12 eV (500°C) to 2.09 eV (700 °C). The experimental results indicate that the evaporation rate (ER) of TiO2-700 °C improved about 17.5% than primary literature, with ER of 0.94 1.62, 1.8 and 2.28 kg m-2 h-1 under 1sun, 2sun, 3sun and 4sun, respectively. This project highlights that ML strategies can accelerate development of high-performance SPMs for solar water evaporation, improving efficiency of seawater desalination.

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