Discovery of FAZnF3, a Hybrid Organic-inorganic Perovskite for Photocatalytic Water Splitting

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The world’s unsustainable reliance on fossil fuels prompts the intense search for innovation to enable paradigm shift to renewable energy. A promising solution is to harness abundant solar energy through photoelectrochemical water splitting to produce hydrogen. However, a major challenge is finding efficient large band-gap crystalline semiconductors to accompany silicon in a tandem water-splitting device. This project combines state-of-the-art random forest machine learning models (ML) with first-principles density functional theory (DFT) quantum mechanical computations to discover promising new hybrid organic-inorganic perovskites (HOIPs). To train the ML model, the researcher compiled geometric and electronic features for 187 distinct HOIPs with ABX3 stoichiometry, where A is a monovalent organic cation, B is a divalent metal cation, and X is a halide. After attaining a coefficient of determinations (R2) of 91% and 85% for band gap and relative energy, respectively, the trained ML models were applied to 1,061 previously unidentified HOIPs to determine the top candidates that exhibit band gaps around 1.6 - 1.8 eV and high thermochemical stability. DFT computations on formamidinium zinc fluoride, HC(NH2)2ZnF3 (abbreviated as FAZnF3), confirmed its potential applicability as the large band gap catalyst in tandem photoelectrochemical water splitting devices for hydrogen production. A literature search reveals that FAZnF3 is previously undiscovered and truly groundbreaking with regards to optimal electronic properties, low toxicity, and relatively high environmental stability.

Awards Won:
Third Award of $1,000