

# Discovery of FAZnF<sub>3</sub>, a Hybrid Organic-inorganic Perovskite for Photocatalytic Water Splitting

Yang, Kaien (School: Thomas Jefferson High School for Science and Technology)

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 ABX<sub>3</sub> 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 (R<sup>2</sup>) 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(NH<sub>2</sub>)<sub>2</sub>ZnF<sub>3</sub> (abbreviated as FAZnF<sub>3</sub>), confirmed its potential applicability as the large band gap catalyst in tandem photoelectrochemical water splitting devices for hydrogen production. A literature search reveals that FAZnF<sub>3</sub> 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