Leveraging State-of-the-Art Machine Learning Models for Bimetallic Catalyst Discovery

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We present a study utilizing state-of-the-art machine learning (ML) models [1] to identify bimetallic transition metal alloys as promising catalysts for the H_2 dissociation reaction. Building on established research demonstrating that bimetallic alloys with density of states (DOS) patterns similar to palladium (Pd) exhibit comparable catalytic performance [2], we employed this descriptor as the basis for high-throughput screening.

Using existing ML models optimized for materials property prediction, we identified candidate alloys with Pd-like DOS characteristics. These predictions were validated against density functional theory (DFT) calculations performed with VASP to ensure consistency and reliability. By focusing on the DOS similarity to Pd [3], a well-known catalytic benchmark, our approach effectively prioritized alloys with high potential for H_2 dissociation. This study underscores the power of integrating ML with experimentally validated descriptors to accelerate the discovery of cost-effective catalytic materials while maintaining rigorous computational accuracy.

[1] Riebesell J, Goodall R E, Jain A, Benner P, Persson K A and Lee A A 2023 *arXiv preprint arXiv:2308.14920*

[2] Yeo B C, Nam H, Nam H, Kim M C, Lee H W, Kim S C, Won S O, Kim D, Lee K Y, Lee S Y *et al.* 2021 *npj Computational Materials* **7** 137

[3] Hammer B, Hansen L B and Nørskov J K 1999 *Physical review B* **59** 7413