Gap: Experimental verification of high-throughput computations

- Battery materials
- Electrocatalytic materials
- Photovoltaic materials
- Gas-separation materials
- Quantum materials
- Thermoelectric materials
- Photocatalytic materials
- Optoelectronic materials
- Magnetic materials
- Piezoelectric materials
- Dielectric materials
- Other materials

Exploring the materials combinatorial space to narrow down candidate selection

High-throughput publications with validation experiments
High-throughput publications without validation experiments

Xiong et al., *Energy Environmental Science* 14, 2335-2348 (2021)
DMREF approach: Integrated computational-experimental discovery cycle

1. Chemical stability
2. Solar absorption
3. Band alignment
4. Corrected band alignment
5. Synthesizability from literature
6. Abundance
7. Phase purity
8. Photocatalytic activity

1. \( \Delta H_f < 0 \text{ eV} \)
2. \( 0.75 < \varepsilon_g < 2 \text{ eV} \)
3. \( E_{VB} > 0.55 \text{ V vs. RHE} \)
4. \( E_{CB} < 0.65 \text{ V vs. RHE} \)
5. \( {L_{50}} > 250 \text{ mg/kg} \)
6. Literature evidence of synthesizability
7. \( E_{VB} > 1.2 \text{ V vs. RHE}, E_{CB} < 0 \text{ V vs. RHE} \)
8. Phase purity confirmed by X-ray diffraction

Xiong et al., Energy Environmental Science 14, 2335-2348 (2021)
Katz et al., Advanced Energy Materials 2201869 (2022)