SI2-SSI: Collaborative Research: A Robust High-throughput Ab initio Computation and Analysis Software Framework for Interface Materials Science

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OBJECTIVES

THE SCIENTIFIC GOAL

- Background: compared to the extensive computational research efforts on the bulk materials, the fundamental understanding and design of materials interfaces with target properties is one of the greatest challenge in the materials science.
- We aim to develop a robust high-throughput *ab-initio* computation and analysis software framework for interface materials science.

THREE FOCUSE RESEARCH AREAS

1. To develop an automated algorithm and software for building grain boundary structures (YANG)
2. To develop a software package to carry out ab-initio thermodynamics of surfaces and interfaces (ONG)
3. To develop advanced methods for materials kinetics and diffusion at materials interfaces (MO)

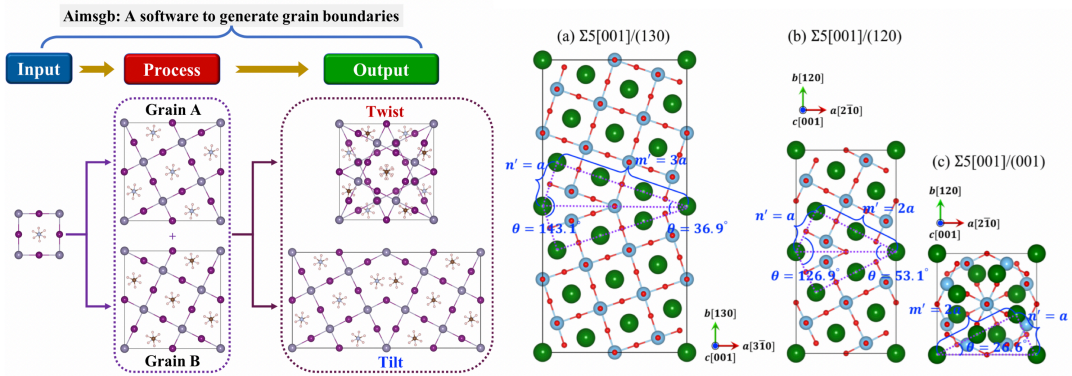
TECHNICAL APPROACH

Developing the proposed software package in python language based on the existing *pymatgen*, *pymatgen-db*, custodian, and Fireworks software libraries, integrating them into a user-friendly and flexible software for *ab-initio* computations and analysis.

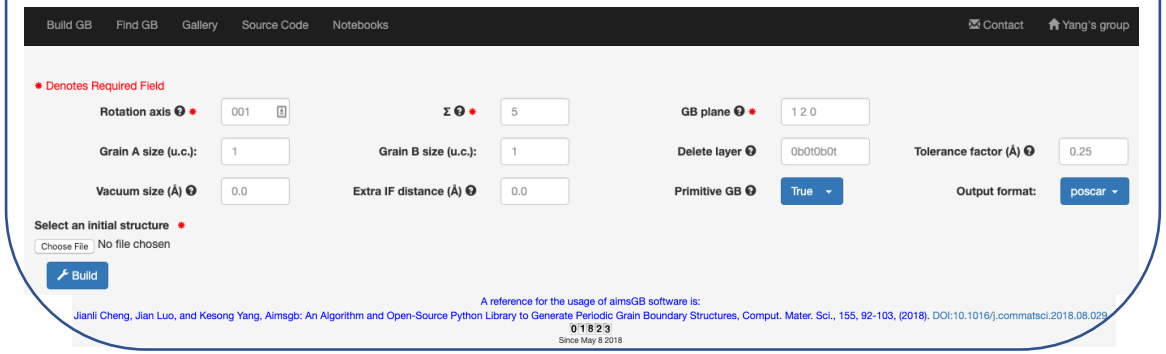
BROAD IMPACTS

- Enable high-throughput investigation and design of novel materials interfaces
- A critical component of the Materials Genome Initiative, along with the existing research efforts for bulk materials
- Educate and train next-generation workforce for Materials Genome Initiative
- **20+ publications**, including J. Chen & K. Yang et al., ***Comput. Mater. Sci.***, 155, 92-103, (2018); Y. Li and K. Yang, ***Energy Environ. Sci.***, 12, 2233-2243, (2019); Y. Chen & K. Yang et al., ***Nature***, 577, 209-215, (2020).

Aimsgb: An Algorithm and Open-Source Python Library to Generate Grain Boundary Structures



A Web-based Application Framework (aimsgb.org)



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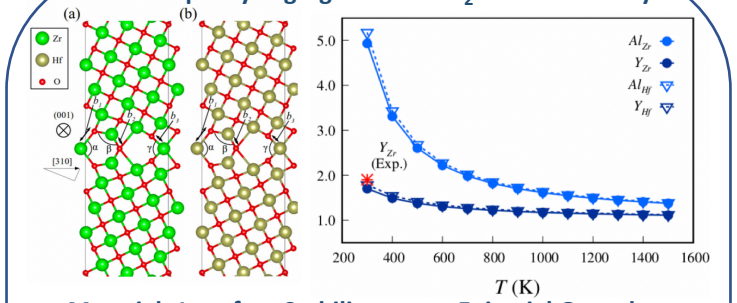
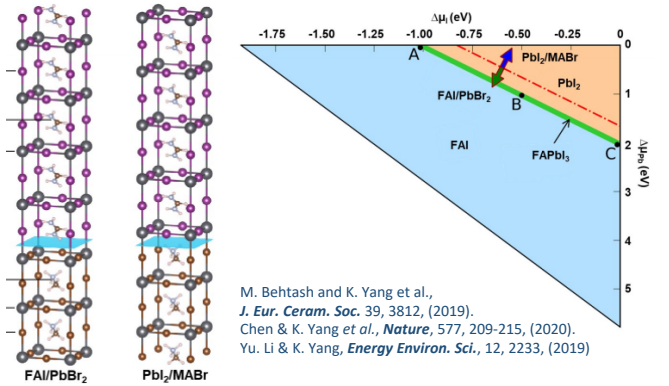
Impurity Segregation at ZrO_2 Grain Boundary

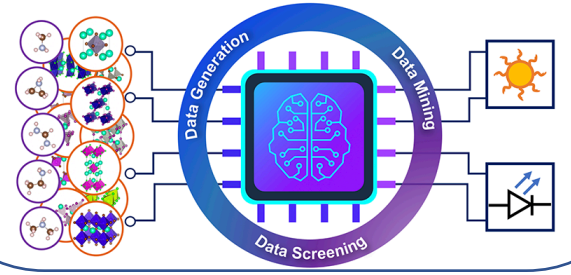


Materials Interface Stability versus Epitaxial Growth



M. Behtash and K. Yang et al., ***J. Eur. Ceram. Soc.*** 39, 3812, (2019).
Chen & K. Yang *et al.*, ***Nature***, 577, 209-215, (2020).
Yu. Li & K. Yang, ***Energy Environ. Sci.***, 12, 2233, (2019)

High-throughput Design of Hybrid Semiconductors



NSF CSSI PI Meeting, Seattle, WA, Feb. 13-14, 2020