Multiscale Computational Mechanics & AI for Materials Design

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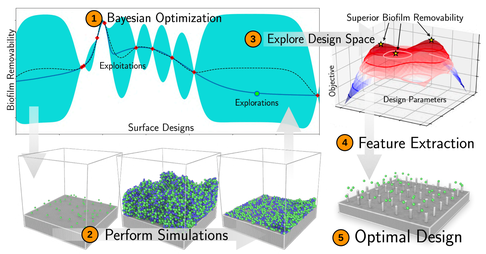
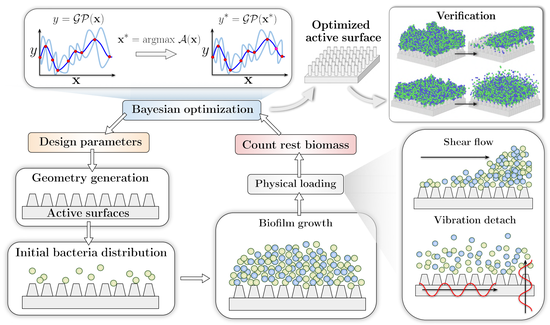
Research Overview & Objective

- We are developing digital material technologies to tackle problems in biomedical, energy, semiconductors, soft robotics, and many more, with a specific interest in biomechanics problems.
- We utilize computational materials science, multiscale mechanics, machine learning, and design optimization to tackle these problems by performing simulations on our supercomputers.
- Our works contribute towards the fundamental understanding of materials behavior, design principles, and computational modeling, with broad impacts in both academia and industry.

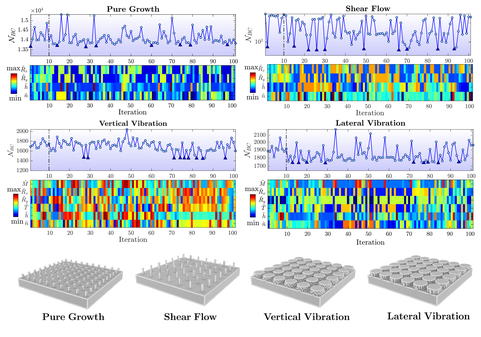
Bayesian Optimization for Antimicrobial Surface Design



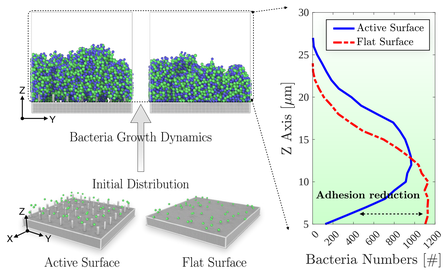
We hope to design nano/micro surfaces to resist biofilm attachment using computer simulations and machine learning techniques.



We developed Bayesian optimization algorithms to generate optimal designs from simulations.



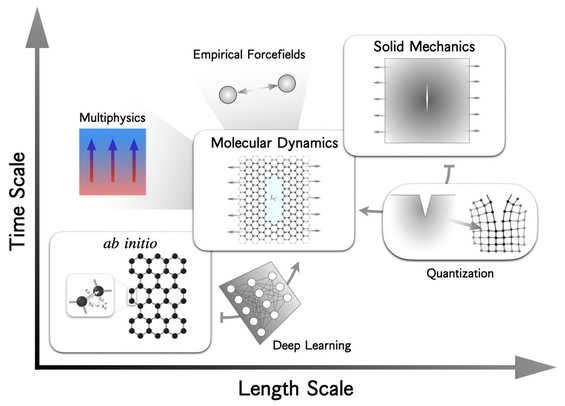
Our framework has successfully extracted optimal surface designs from automated simulations



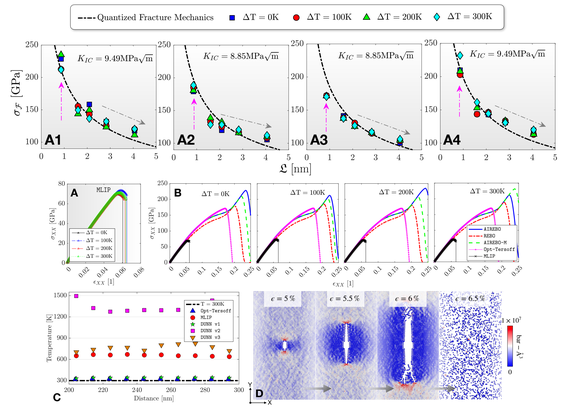
Based on our optimization results, we provide explanations of the biofilm removal mechanisms by looking at the adhesion mechanics.

← Scan the QR code to read the paper.
This work is published on *ACS Biomaterials Science & Engineering*.

Scale-Bridging for Graphene Fracture Mechanics



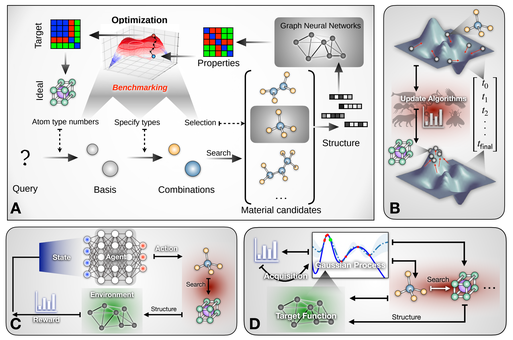
We hope to understand the multiscale mechanism of the nonequilibrium fracture of graphene.



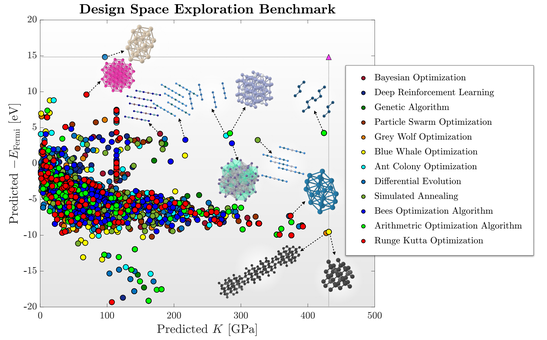
We verify molecular simulation with fracture mechanics theories and benchmark different interatomic potentials with neural network potentials.

← Scan the QR code to read the paper.
This work is under review for *International Journal of Applied Mechanics*.
Previously presented at *Molecular Machine Learning Conference* at MIT.

Benchmarking Inverse Algorithms for Materials Design



We want to benchmark different inverse optimization algorithms for computational materials design.



We examine the exploitation/exploration process of different algorithms and further analyze the optimized molecular materials.

This work is an ongoing collaboration with *Microsoft Research Asia*. Preprint to be released soon.

Future Research & Potential Directions

- Develop and utilize different algorithms to model the complex mechanical behavior of biofilm and engineering living materials.
- Developing machine learning potentials for deploying large-scale molecular simulations under extreme environments.
- Develop inverse optimization algorithms and computational models for socio-resilient materials design.

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