

# AI for Good + AI for Science

*Designing next generation biocompatible materials with Machine Learning + Multiscale & Multiphysics Modeling*

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### Goal & Objective

**Bacteria cells**

**Biofouling**

Biofilm stinks. We hope to find a way to get rid of it. Designing a new kind of nanosurface with computer simulation + ML is one.

### Developed Toolbox

**Bayesian Optimization**

- Design Space & Hyper-parameters
- Gaussian Process Surrogate Model
- Acquisition Function

**Python**

- Design Variables
- Optimization
- Finalize Design

**LAMMPS**

- Digital Twins

**Verification**

- High Fidelity Simulation

**PyLAMDO** depends on the Python-LAMMPS interface for automating the simulation + optimization processes.

### Some Preliminary Results

Inferring biomass from roughness

**A Prediction on Test Data**

**B Prediction on "Unseen" Data**

### Methodology

#### Mesoscale Modeling

Mesoscale modeling (i.e. DEM) accounts complex physics information.

#### Bayesian Optimization

Bayesian optimization is a powerful tool in materials design.

#### Operator Learning

DeepONet can learning the mapping between functional spaces.

### Surrogate model – based designing

Original Field

One-Shot LUC

Surrogate Model  $\hat{M}$

Detailed Field

Optimized Antimicrobial Surface Design

Final Metamodel  $\hat{M}$

Find Field Minimum

Refined Surrogate Model  $\hat{M}$

One-Shot LUC