# AI for Materials Science: Tuning Laser-Induced Graphene Production and Beyond


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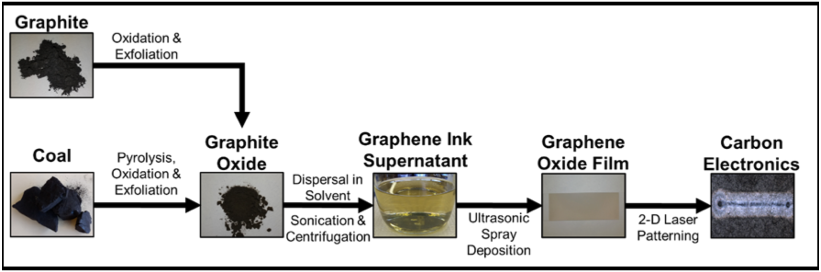
NASA Ames, 29 October 2019

# From Graphite/Coal to Carbon Electronics



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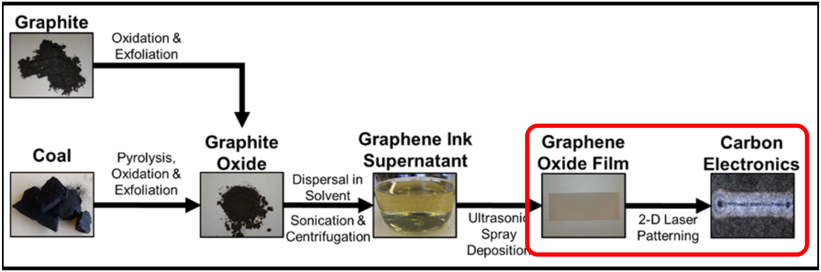
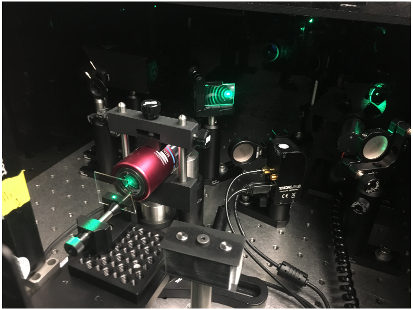
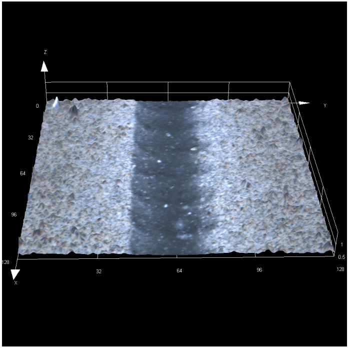


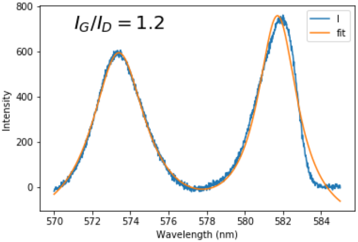
# Optimizing Graphene Oxide Reduction

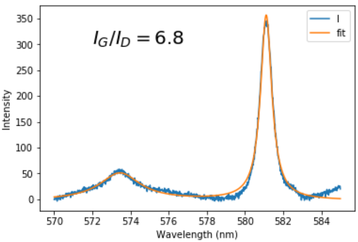
- reduce graphene oxide to graphene through laser irradiation
- allows to create electrically conductive lines in insulating material
- laser parameters need to be tuned carefully to achieve good results



# Evaluation of Irradiated Material



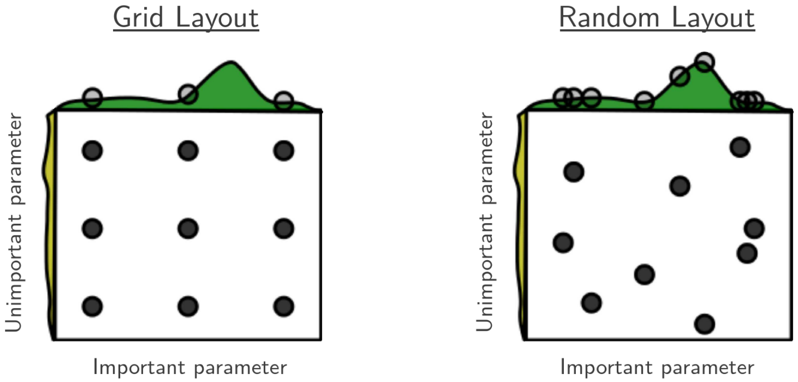
# Laser Parameters

- laser power (1 mW to 4400 mW), duration for irradiating spot (710 ms to 20 210 ms), pressure in reaction chamber (10 psi to 100 psi)
- ≈7.8 billion configurations
- individual graphene oxide sample allows for max 361 evaluations, about 2 weeks of human operator time

# Automated Parameter Tuning

- treat tunable process as black box
- no knowledge of inner workings required – no first-principles understanding of how graphene oxide reduction works
- evaluate different parameter settings to identify performance improvements
- mature techniques used in many areas of AI and elsewhere

# Grid and Random Search

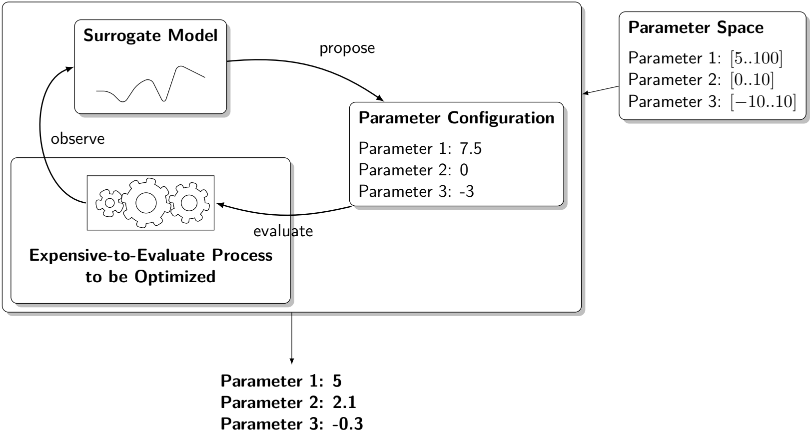



Bergstra, James, and Yoshua Bengio. "Random Search for Hyper-Parameter Optimization." J. Mach. Learn. Res. 13, no. 1 (February 2012): 281–305.

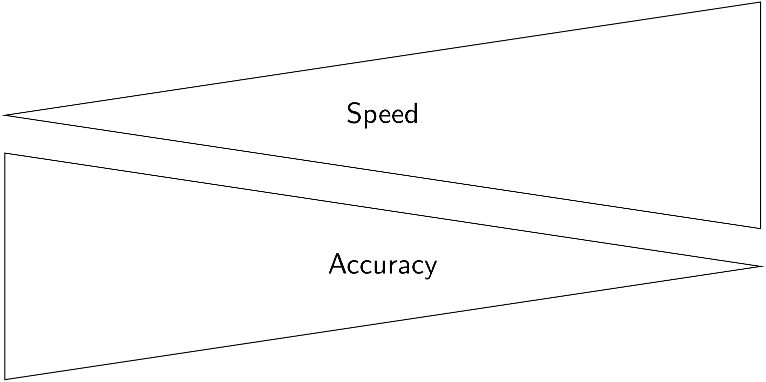
# Bayesian Optimization with Surrogate Models

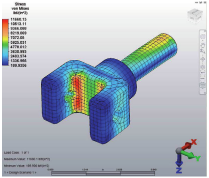
- evaluate small number of initial (random) configurations
- build surrogate model of parameter-performance surface based on this
- use model to predict where to evaluate next
- repeat
- allows targeted exploration of new configurations

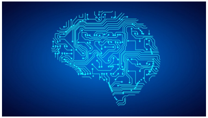
# Bayesian Optimization with Surrogate Models

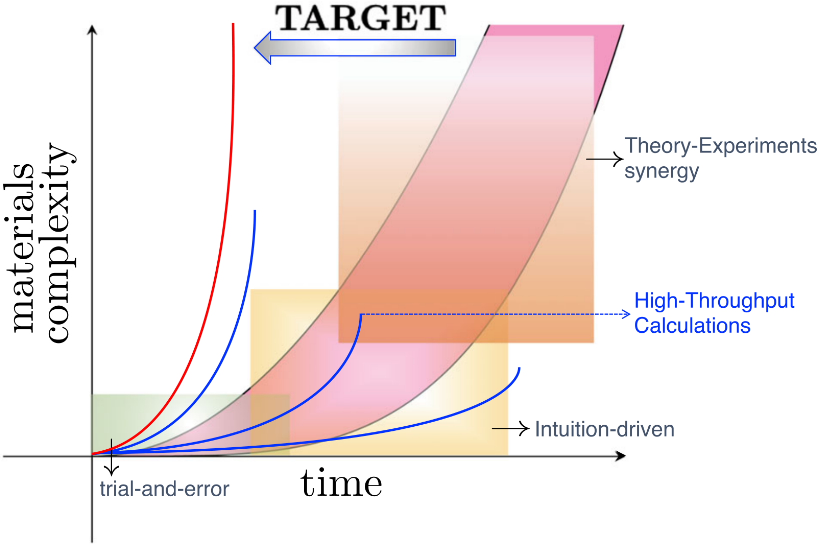


# Surrogate Models






Lookman, Turab, Prasanna V. Balachandran, Dezhen Xue, and Ruihao Yuan. "Active Learning in Materials Science with Emphasis on Adaptive Sampling Using Uncertainties for Targeted Design." Npj Computational Materials 5, no. 1 (February 18, 2019): 21. https://doi.org/10.1038/s41524-019-0153-8.

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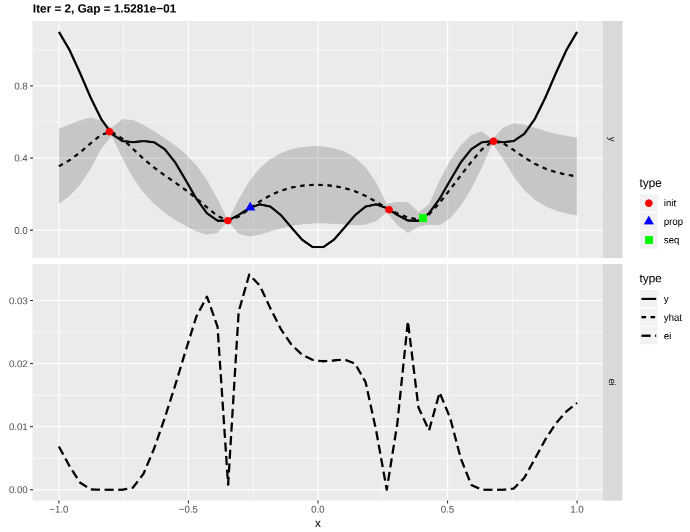


Bischl, Bernd, Jakob Richter, Jakob Bossek, Daniel Horn, Janek Thomas, and Michel Lang. "MlrMBO: A Modular Framework for Model-Based Optimization of Expensive Black-Box Functions," March 9, 2017. http://arxiv.org/abs/1703.03373.

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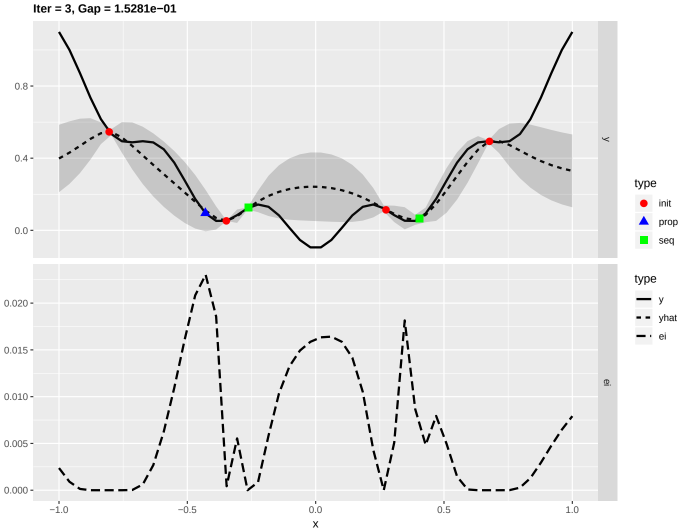


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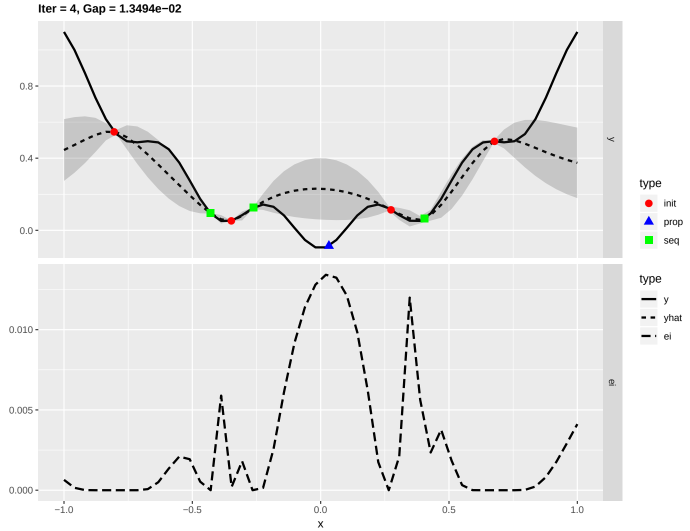


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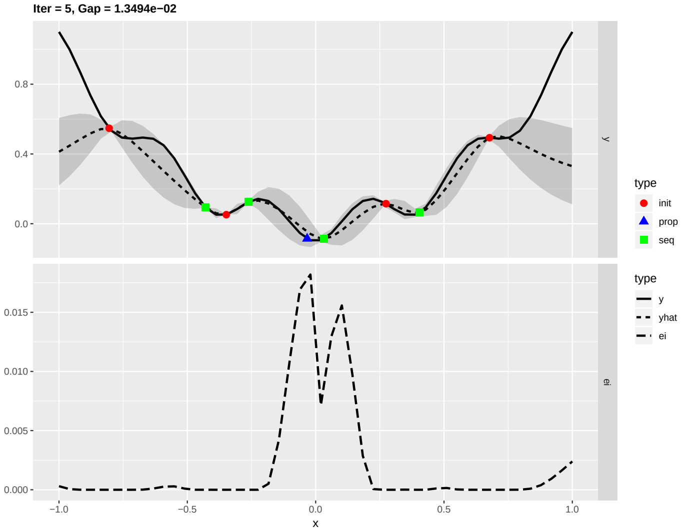


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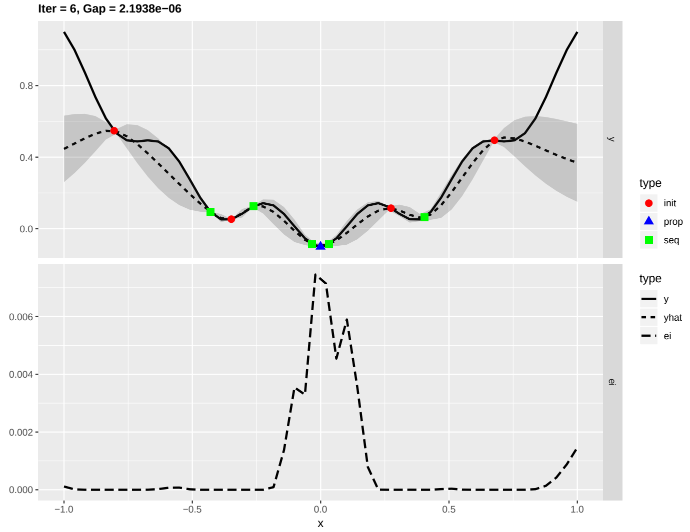


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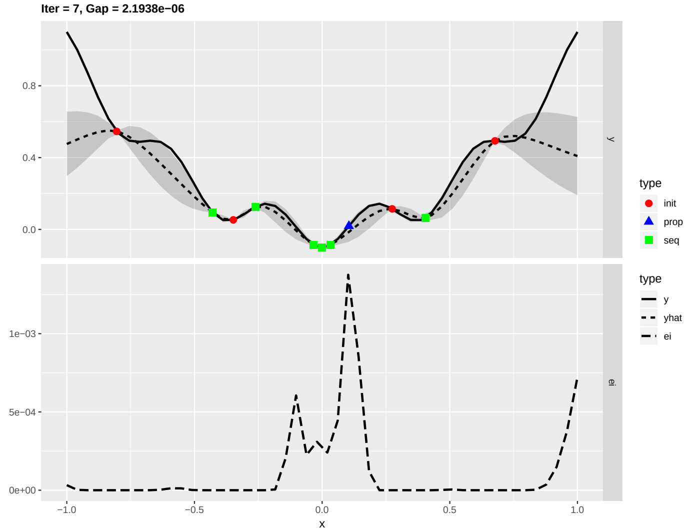


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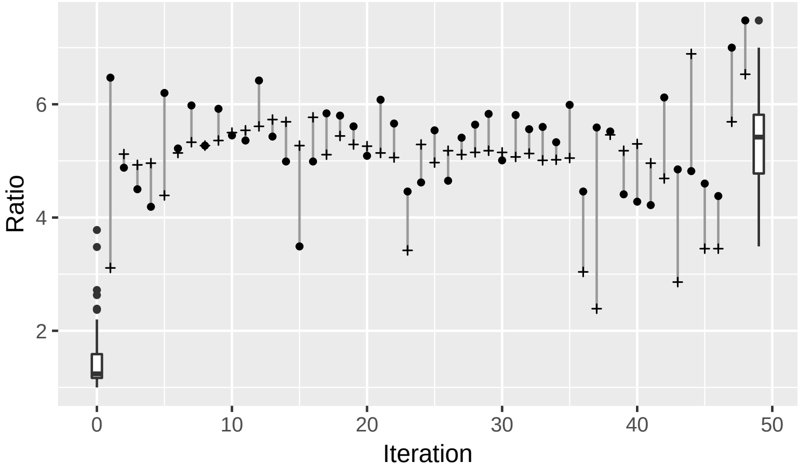
# Tuned Parameters



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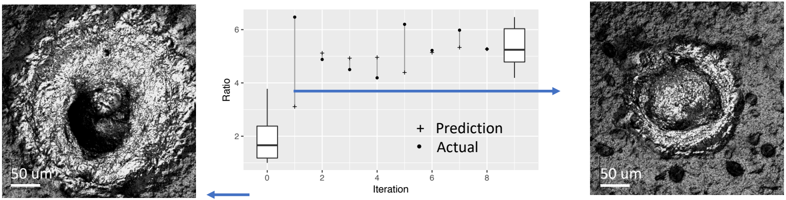
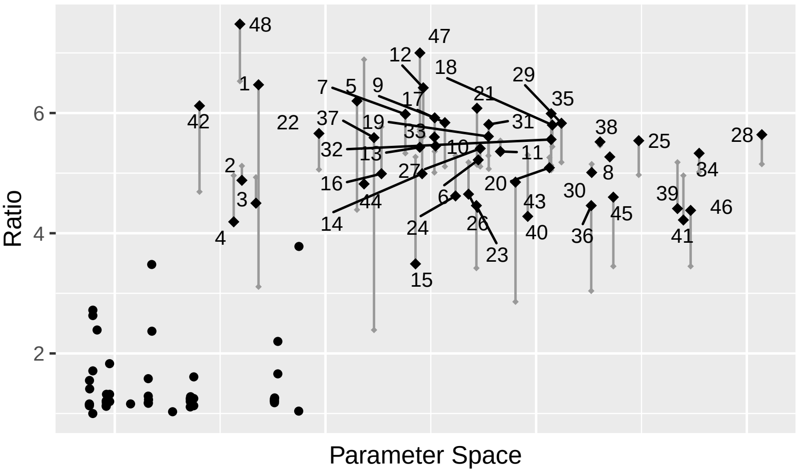



- improvement of factor of two over best result
- good results even with small amount of initial data (19 evaluations)
- code can be used by domain experts with no background in machine learning

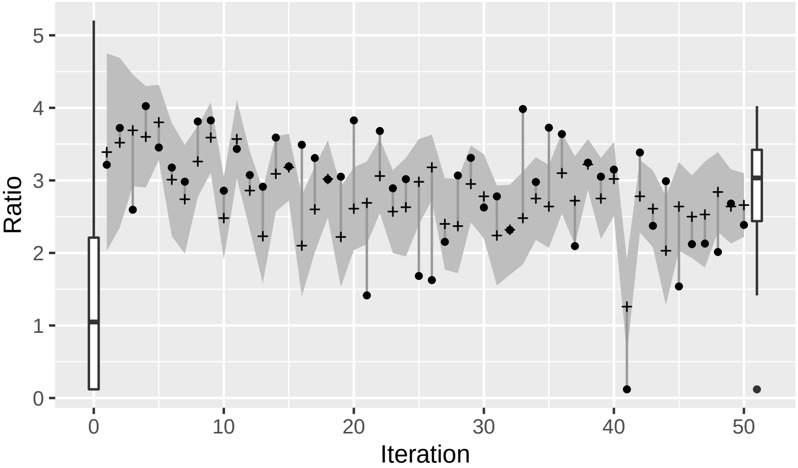
# Explored Parameter Space



# Tuned Parameters – Kapton

- extend parameter space with gas in reaction chamber – air, argon, nitrogen
- extend ranges of other parameters
- more and longer experimental campaigns

# Tuned Parameters – Kapton



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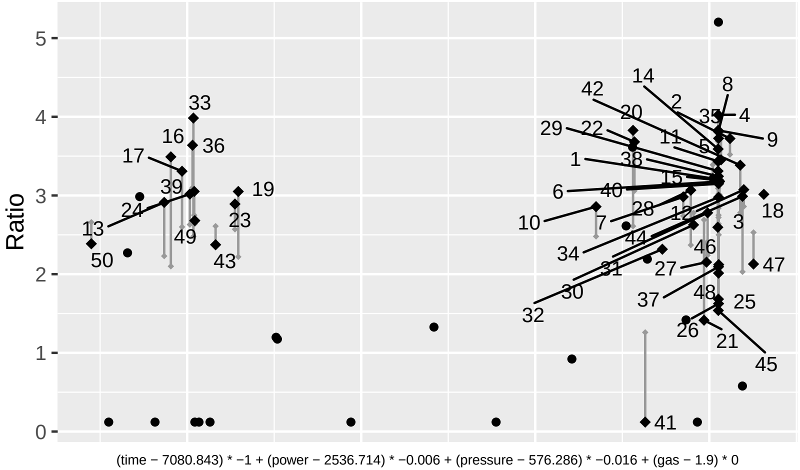
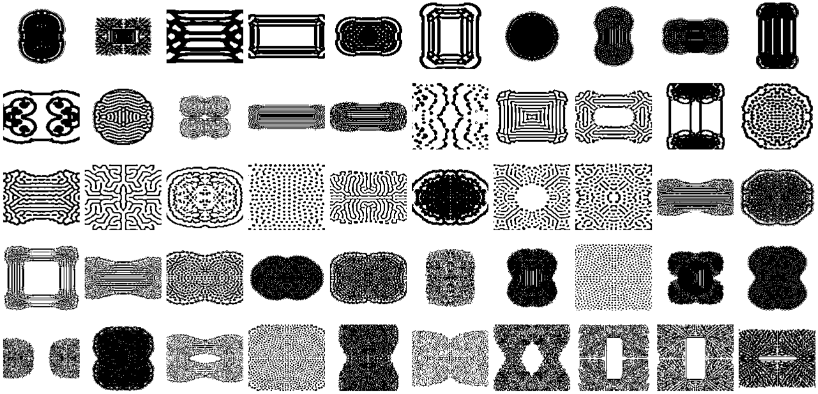
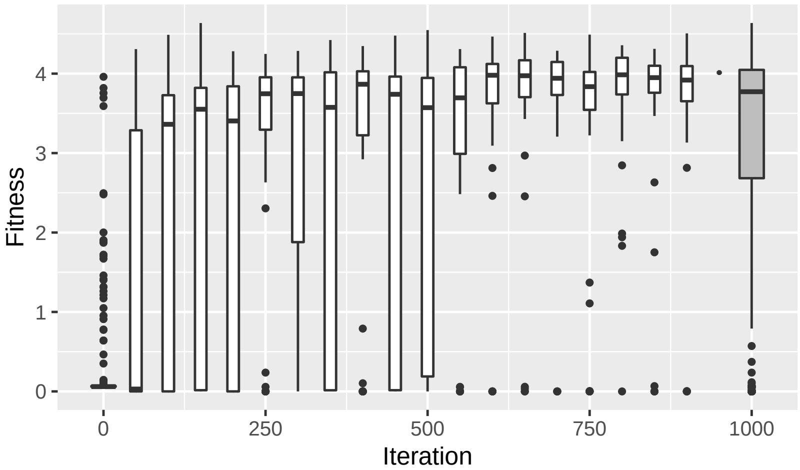


# Design of New Materials



- optimize parameters of pattern generator for energy absorption of material
- six numeric parameters
- computational evaluation of candidates

# ML-Optimized Generator Parameters



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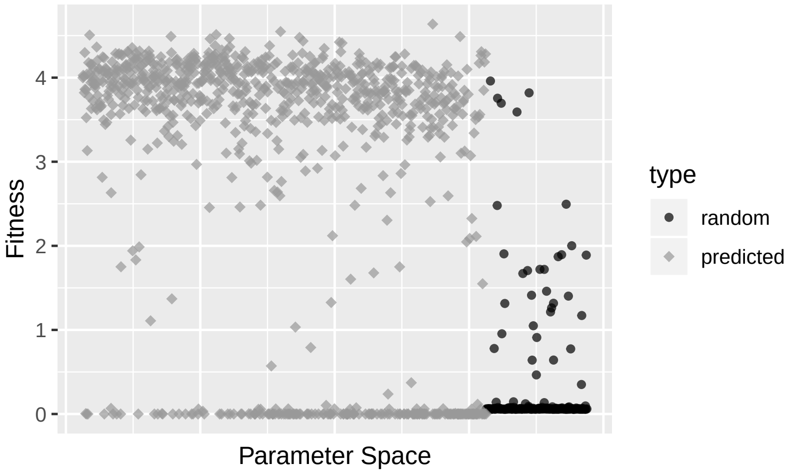

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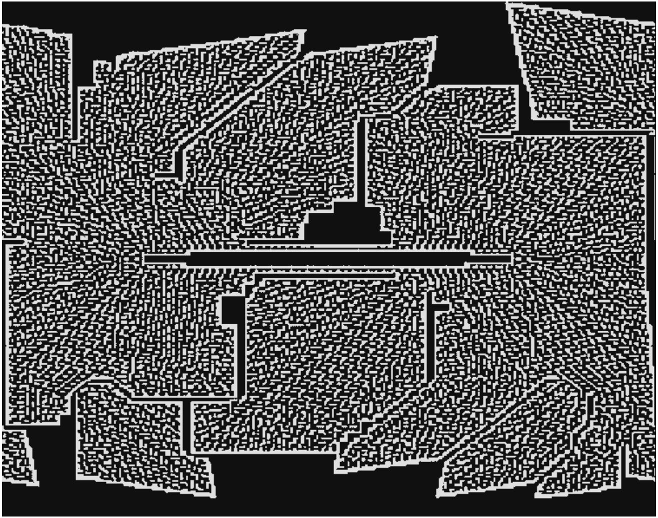


# Outlook

- automate experimental setup
- application to other materials
- more in-depth investigation of Bayesian Optimization performance (and other approaches)
- inform understanding of process by what surrogate model has learned
- additional and multi-scale measurements
- combination of computational simulations (DFT) and experiments
- surrogate models for DFT simulations

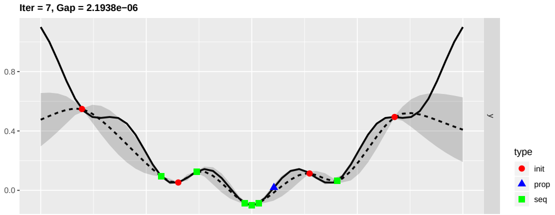
# Similar Approaches

- COMBO: Ueno, Tsuyoshi, Trevor David Rhone, Zhufeng Hou, Teruyasu Mizoguchi, and Koji Tsuda. "COMBO: An Efficient Bayesian Optimization Library for Materials Science." Materials Discovery 4 (2016): 18–21. https://doi.org/10.1016/j.md.2016.04.001.
- Phoenics: Häse, Florian, Loïc M. Roch, Christoph Kreisbeck, and Alán Aspuru-Guzik. "Phoenics: A Bayesian Optimizer for Chemistry." ACS Central Science 4, no. 9 (September 26, 2018): 1134–45. https://doi.org/10.1021/acscentsci.8b00307.
- Matpredict: Talapatra, Anjana, Shahin Boluki, Thien Duong, Xiaoning Qian, Edward Dougherty, and Raymundo Arróyave. "Autonomous Efficient Experiment Design for Materials Discovery with Bayesian Model Averaging." Phys. Rev. Materials 2, no. 11 (November 2018): 113803. https://doi.org/10.1103/PhysRevMaterials.2.113803.
- ...

# Long-Term Outlook

- general framework for surrogate-model-based optimization in materials science
- demonstrate power and flexibility through successful applications in different domains
- build ecosystem and community around framework

# Summary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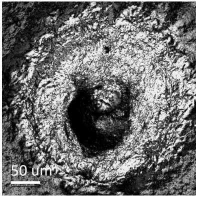
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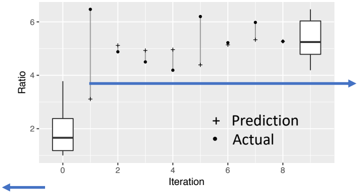
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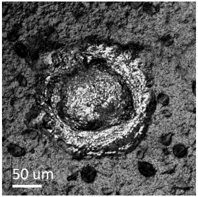
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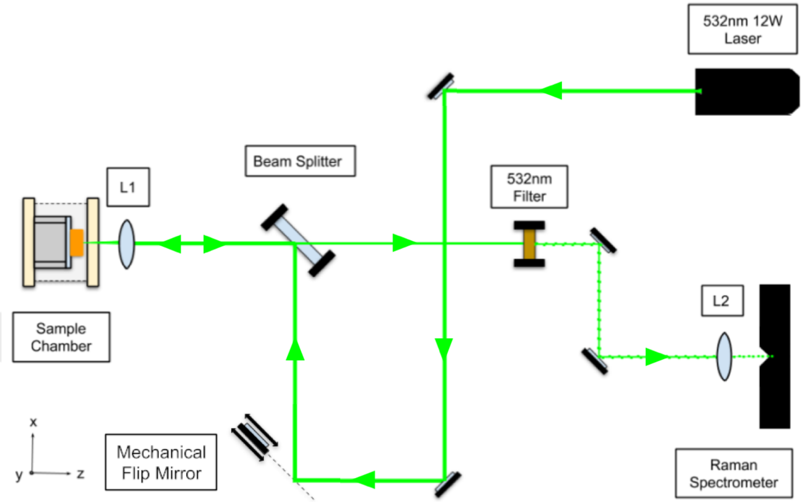
# Experimental Setup



# Morphology of Irradiated Material