Optimization of laser-induced graphene manufacturing

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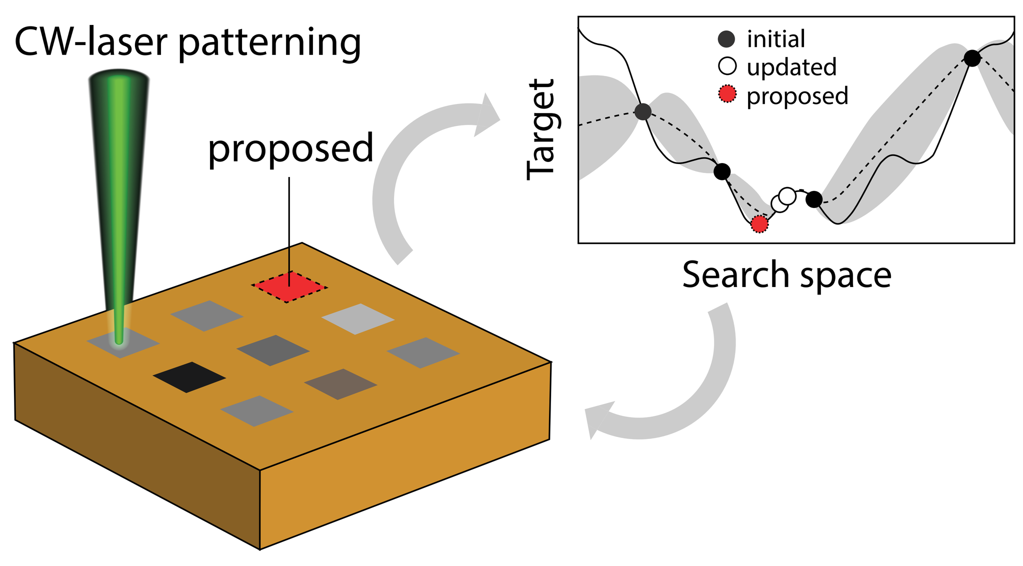
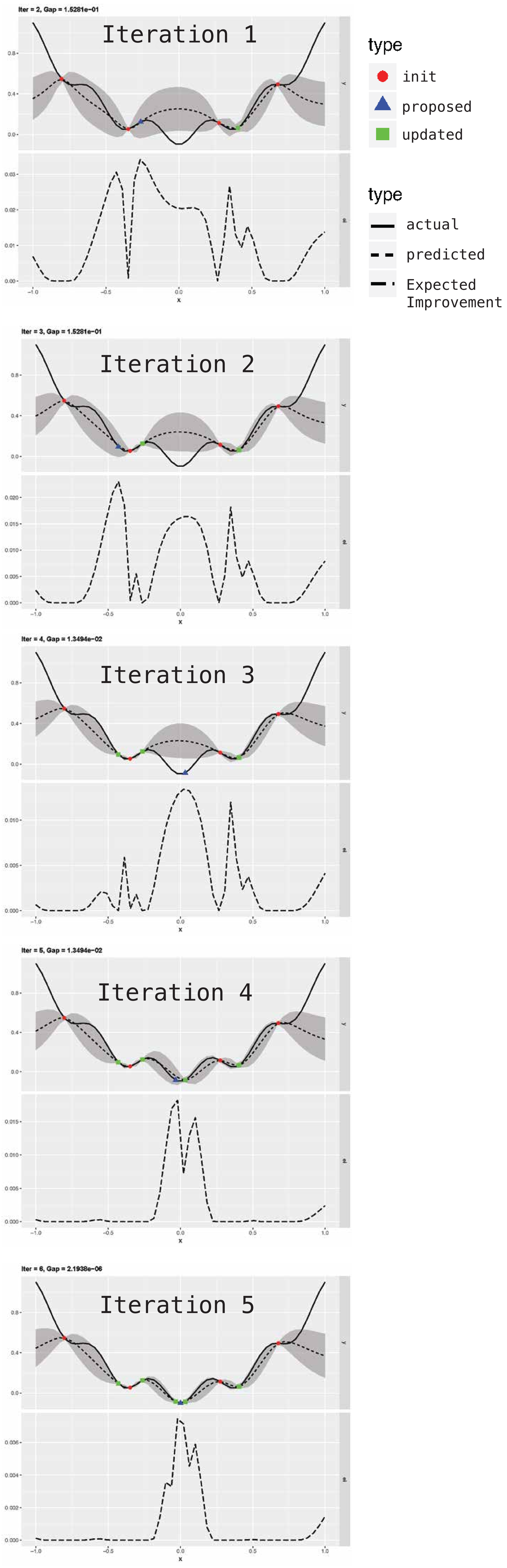
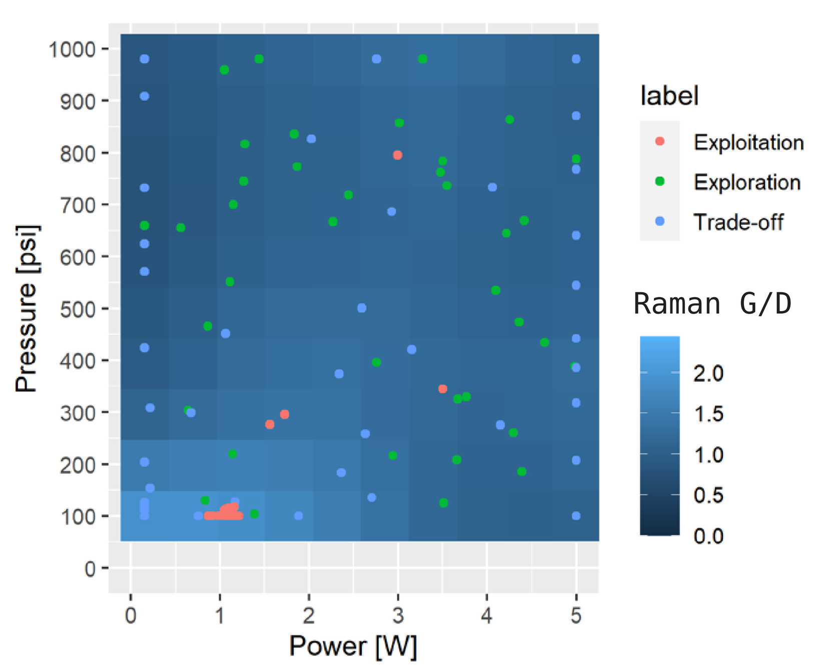
A lot of technological advances depend on next-generation materials, such as graphene, which enables better electronics, to name but one example. Manufacturing such materials is often difficult, in particular, producing graphene at scale is an open problem. We apply state-of-the-art machine learning to optimize the production of laser-induced graphene, an established manufacturing method that has shown great promise. We demonstrate improvements over previous results in terms of the quality of the produced graphene from a variety of different precursor materials. We use Bayesian model-based optimization to quickly improve outcomes based on little initial data and show the robustness of our approach to different experimental conditions, tackling a small-data problem in contrast to the more common big-data applications of machine learning. We analyze the learned surrogate models with respect to the quality of their predictions and learned relationships that may be of interest to domain experts and improve our understanding of the processes governing laser-induced graphene production.



Exploration vs Exploitation

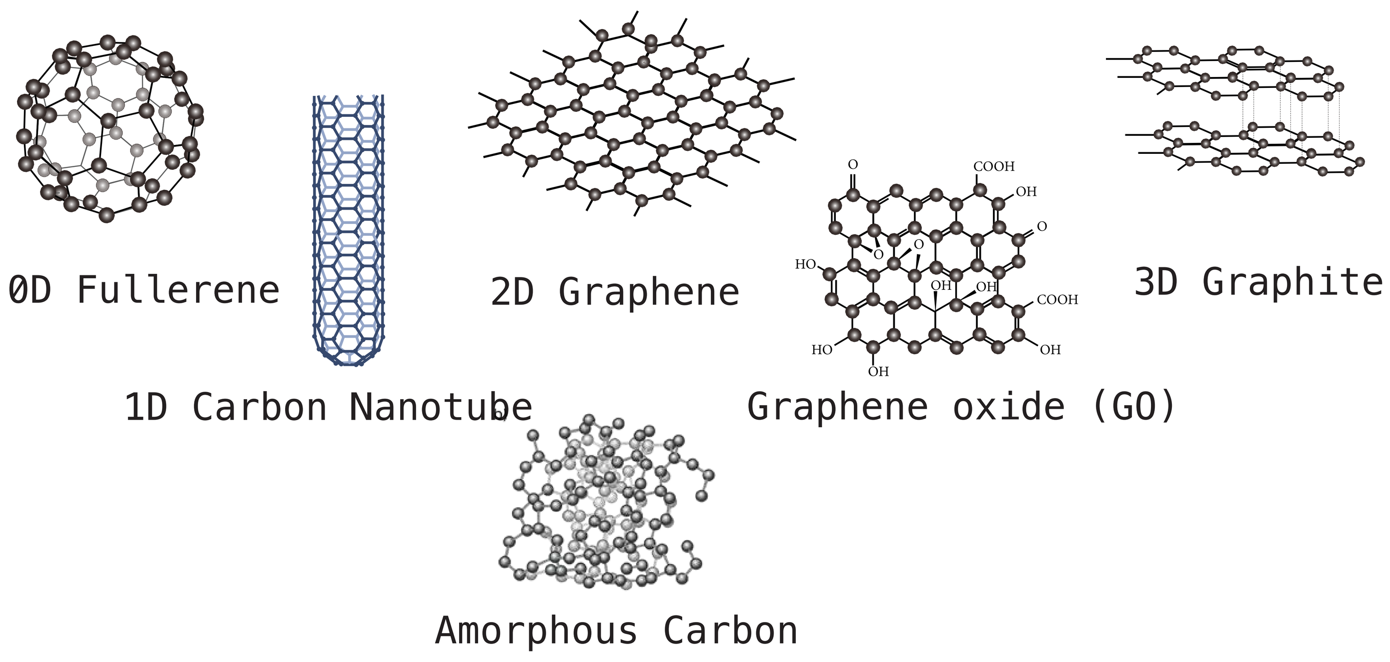


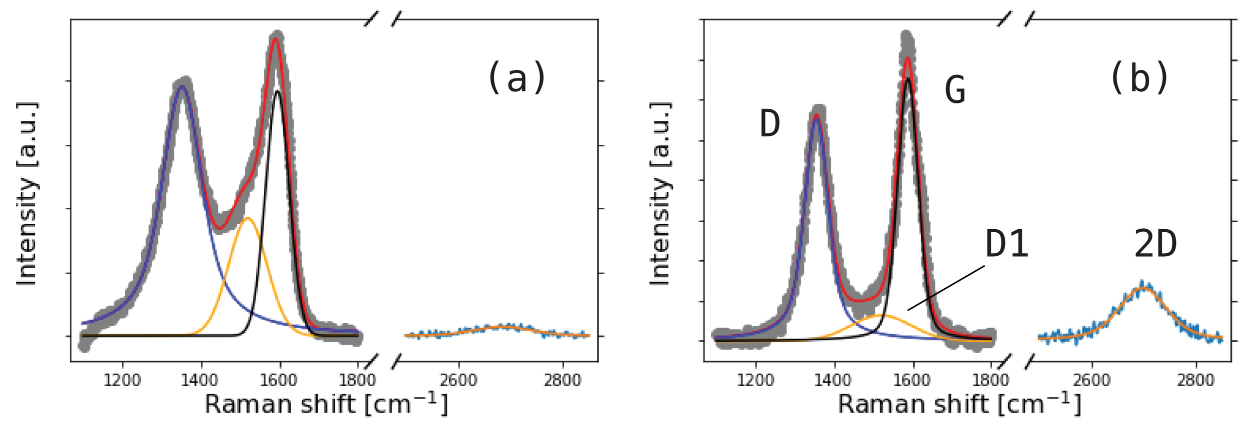
Visualizing how exploration escapes local minima to find the global minima



Comparing exploitation, exploration and trade-offs in a partial dependence plot

Optimization of structural properties





Structural characteristics of LIG (a) before and (b) after patterning of GO. D is attributed to defects. G to in-plane vibrations of sp2 carbon atoms. 2D to stacking order of carbon planes. D1 to amorphous carbon.

Single-step Bayesian Optimization (BO)

BO loop

Require: Search space Λ, cost function c, acquisition function u, predictive model $\hat{c}$, maximal number of function evaluations T

Result : Best configuration $\hat{\lambda}$ (according to $\mathcal{D}$ or $\hat{c}$)

Initialize data $\mathcal{D}^{(0)}$ with initial observations

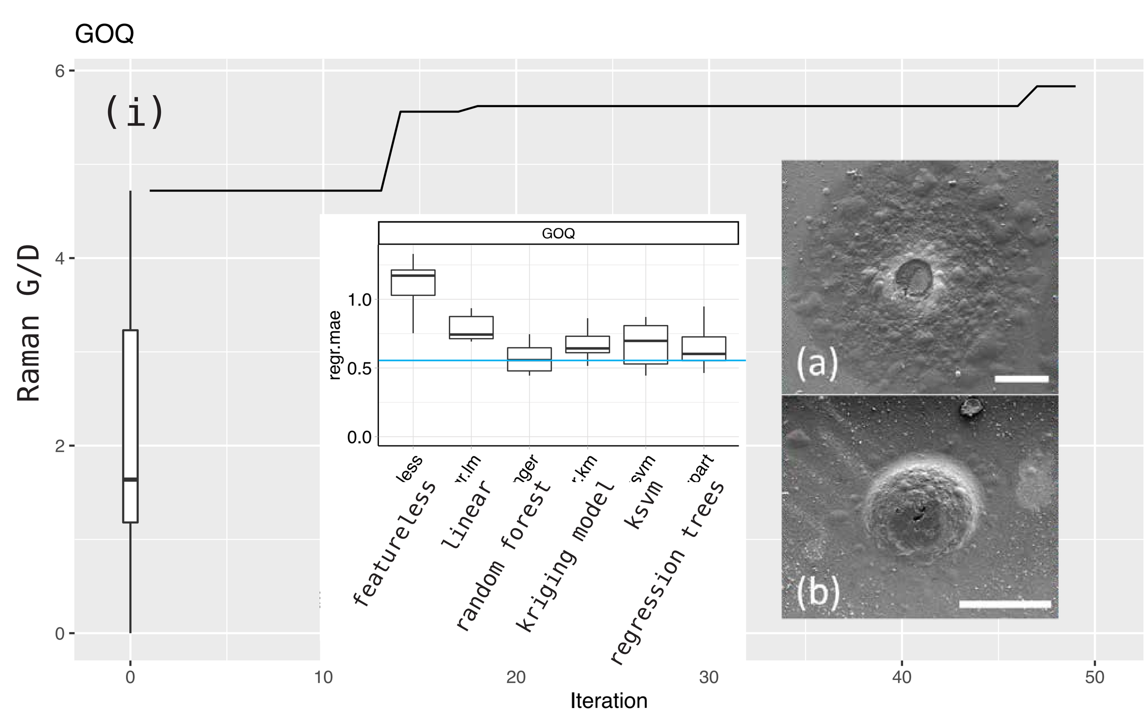
for $t = 1$ **to** T **do**

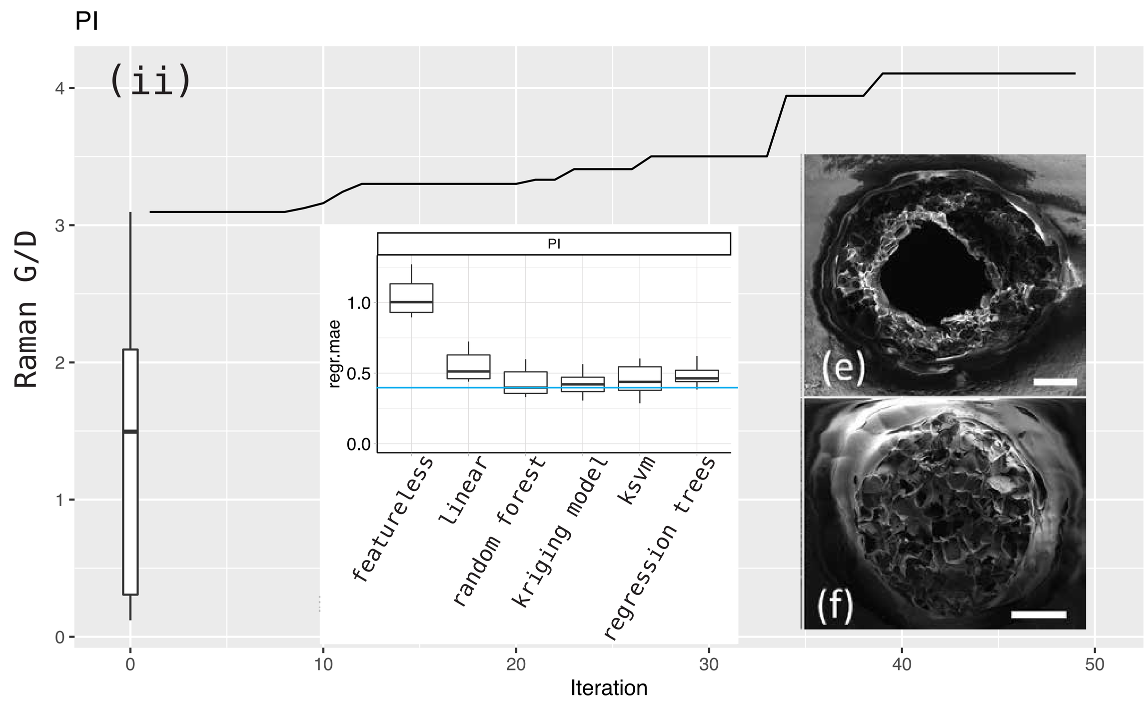
  Fit predictive model $\hat{c}^{(t)}$ on $\mathcal{D}^{(t-1)}$

  Select next query point: $\lambda^{(t)} \in \arg\max_{\lambda \in \Lambda} u(\lambda; \mathcal{D}^{(t-1)}, \hat{c}^{(t)})$

  Query $c(\lambda^{(t)})$

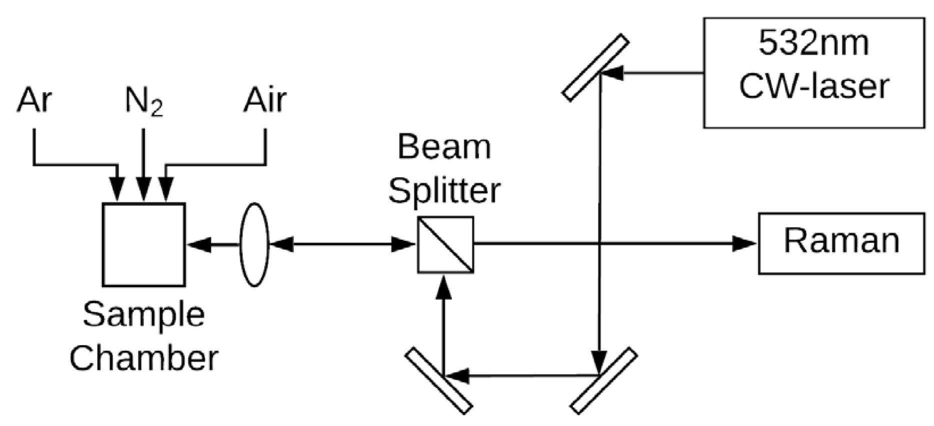
  Update data: $\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \lambda^{(t)}, c(\lambda^{(t)}) \rangle\}$





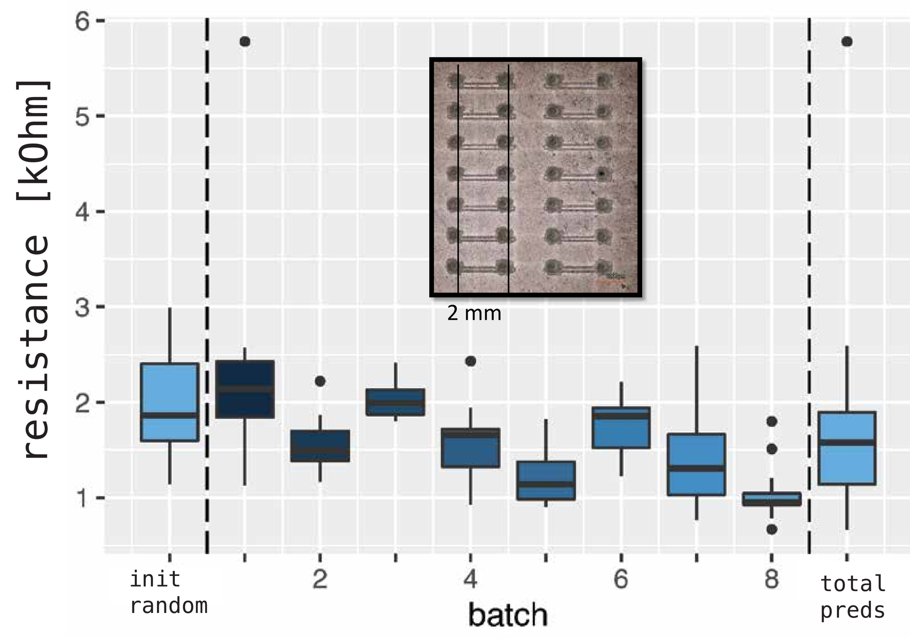
Single-step optimization of the structural quality of LIG on various precursors (i) GO on quartz and (ii) polyimide; higher is better. Boxplot shows distribution of initial training data. Inset: (Left) Comparison of various model performances (right) Scanning electron micrograph of patterned LIG using (a),(e) random and (b),(f) BO parameters

Closed-loop Setup



Optimization of electrical properties

Batch BO

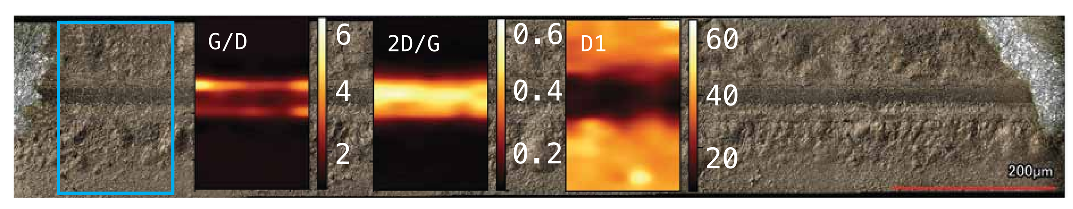


Batch optimization of electrical property of patterned LIG, lower is better.
On the left, the distribution of resistance for the initial training data is shown. Each batch has 14 lines (inset); each boxplot represents one batch. On the right, the distribution of measured resistances for all configurations that the MBO explored.

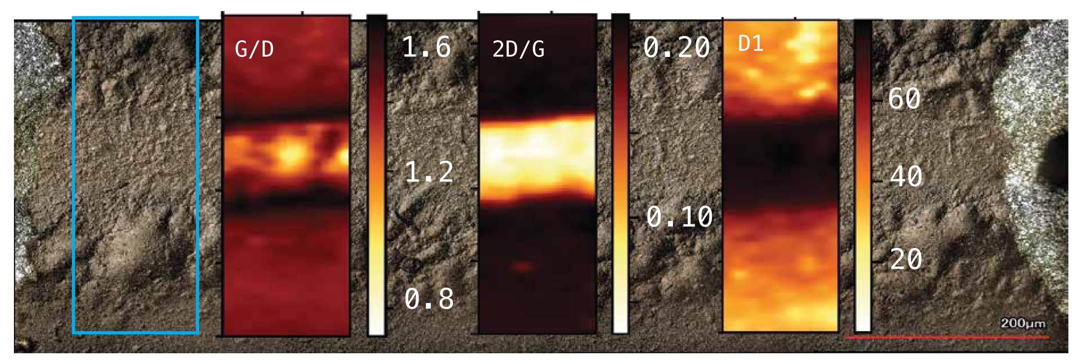
Correlation between structural and electrical properties

variable	correlation	p-value
I(D)	0.744	<= 1e-4
Pos(D)	-0.592	<= 1e-4
Width(D)	0.505	<= 1e-3
I(D1)	0.379	<= 1e-3
I(2D)/I(G)	0.348	<= 1e-3
Width(D1)	-0.206	<= 5e-2
I(G)	-0.176	<= 5e-2

High resistance



Low resistance



Morphology and Raman 2D map of LIG with (a) high and (b) low electrical resistance. Common structures that are characteristic of high-quality graphene (G/D and 2D/G) do not correlate well with resistance; instead, reducing amorphous carbon (D1) does, as evident from the table results. Homogeneity of the structures seem to also play a role in improving electrical property, suggesting that rich data input may improve predictions. Future work would include optimizing a balance between measurement cost and prediction quality.

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https://github.com/aim-uwyo/lig-model-opt

L. Kotthoff,et al, Frontiers in AI and Applications (2022), 31–44
H. Wahab, et al, Carbon 167 (2020) 609–619