



Gr-ResQ

Graphene Recipes for Synthesis of High Quality Materials

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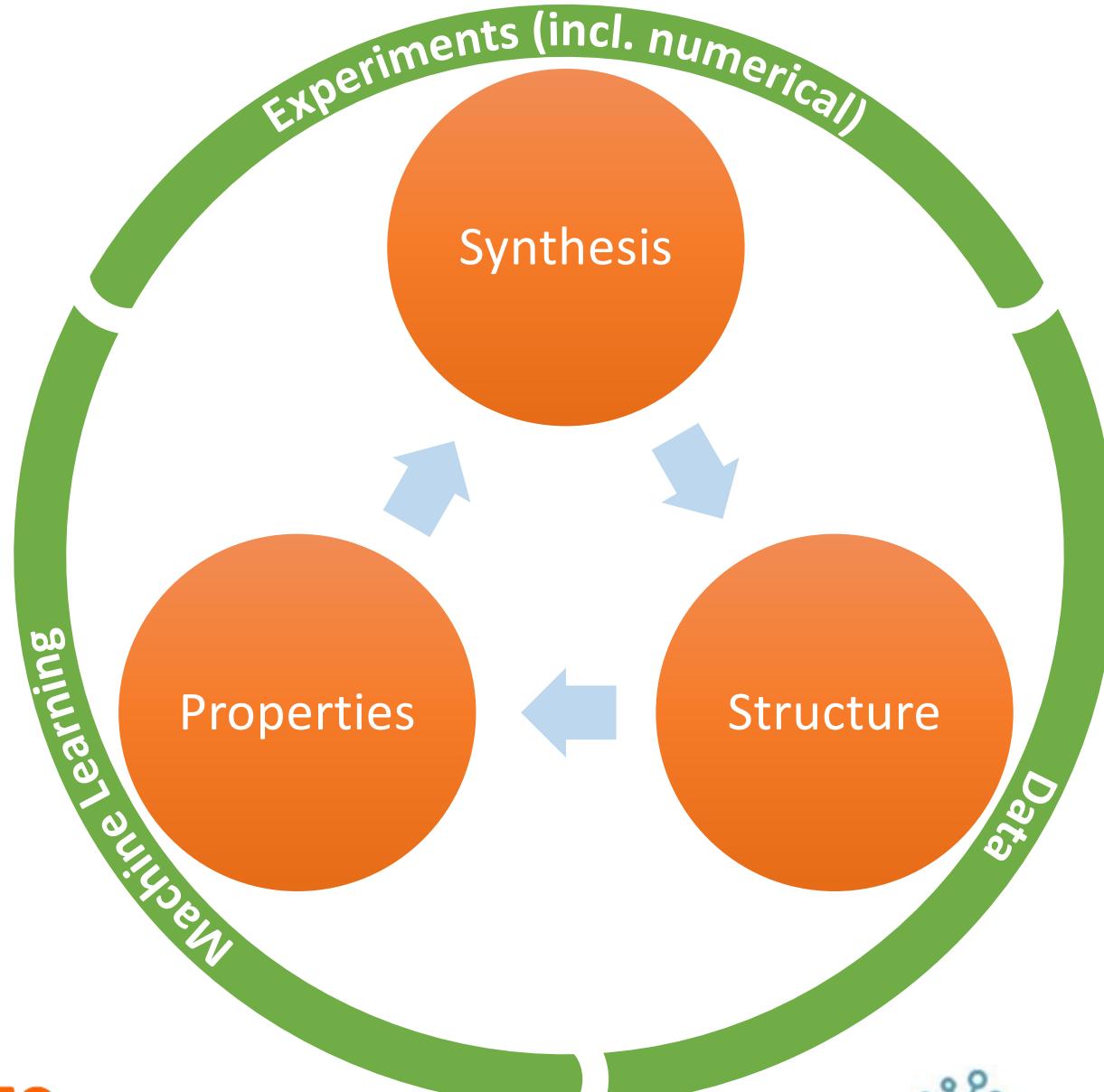
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University of Illinois at Urbana-Champaign



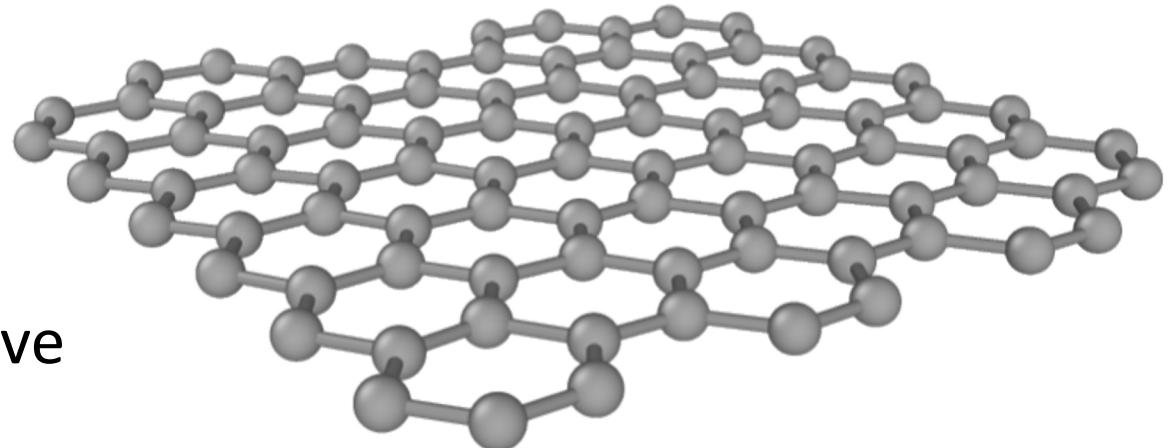
From Rational Design to Data Driven Manufacturing



Graphene

2-dimensional sheet of carbon atoms

“Honeycomb” lattice

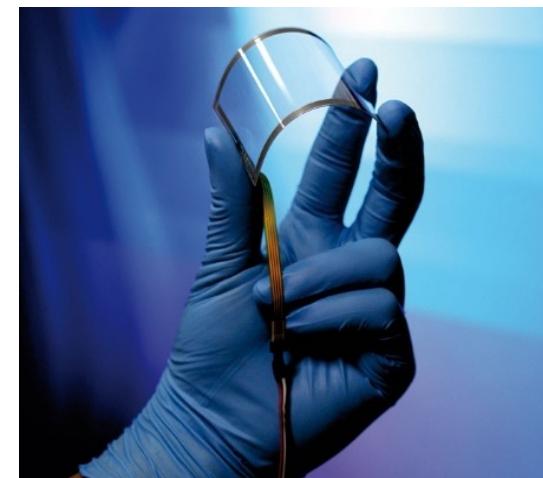


Properties

- High strength
- Electrically conductive
- Lightweight
- Flexible

Applications

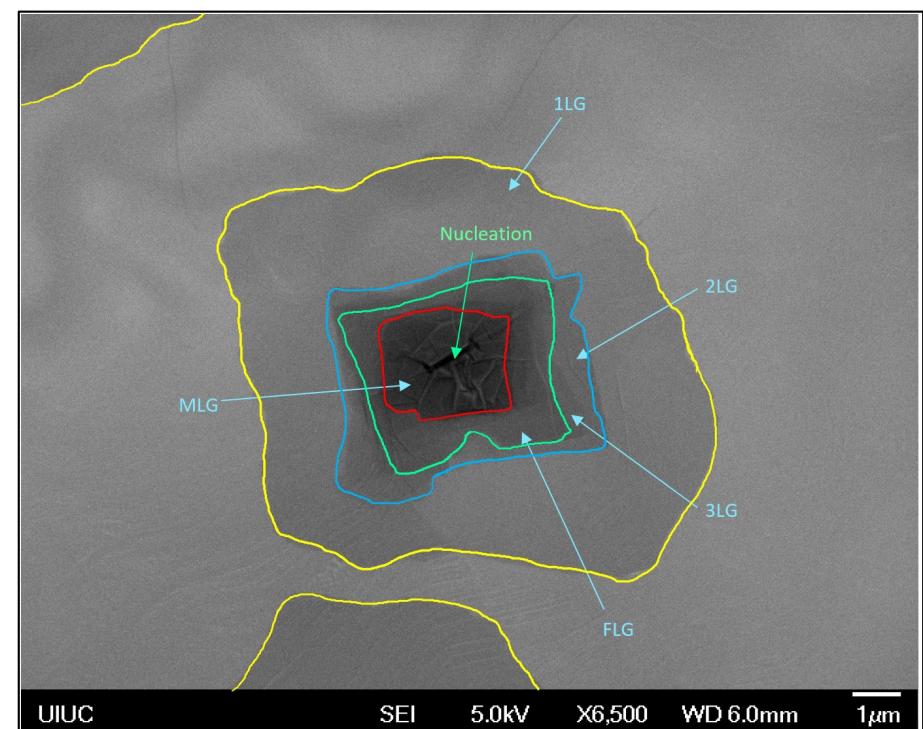
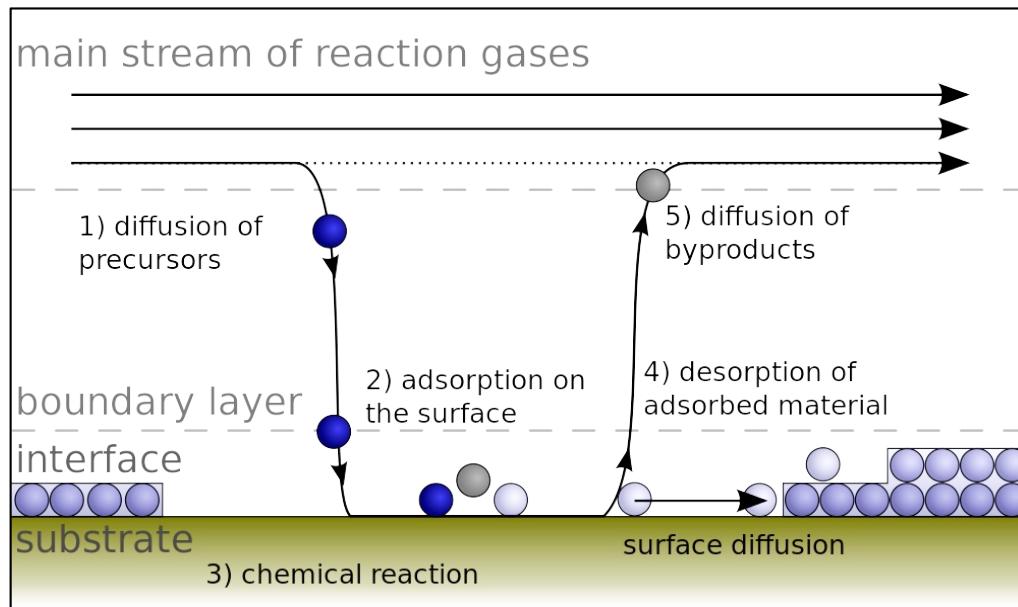
- Transparent conductor
- Flexible electronics
- Mechanical composites



<https://www.nature.com/news/graphene-the-quest-for-supercarbon-1.14193>

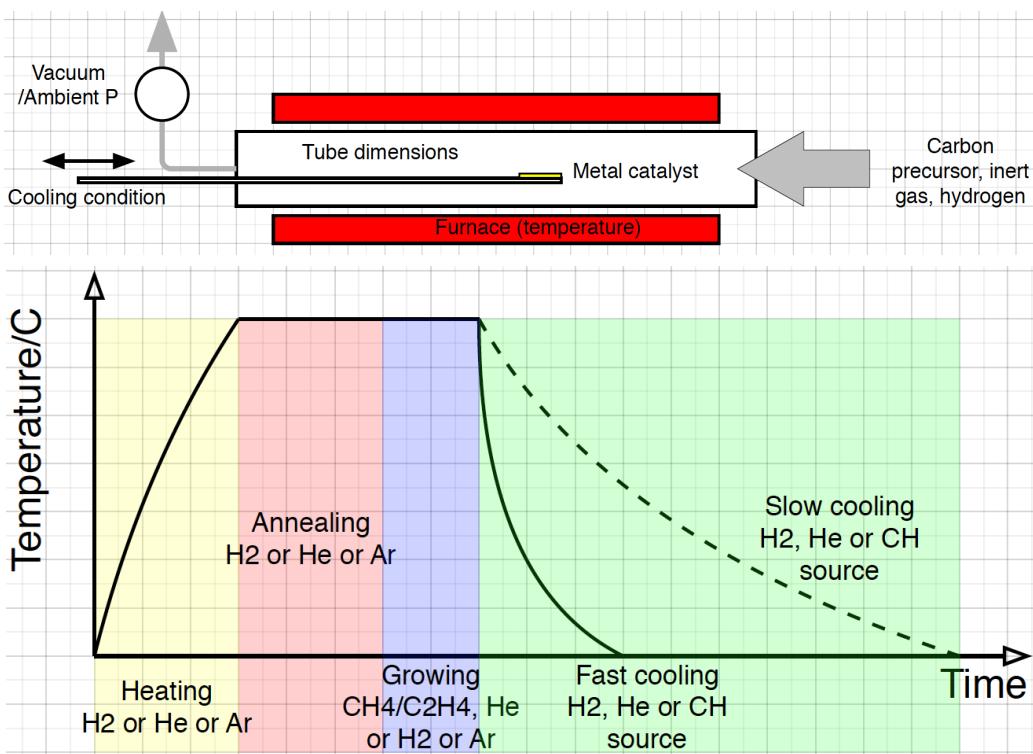
Graphene Synthesis

How do we make it?



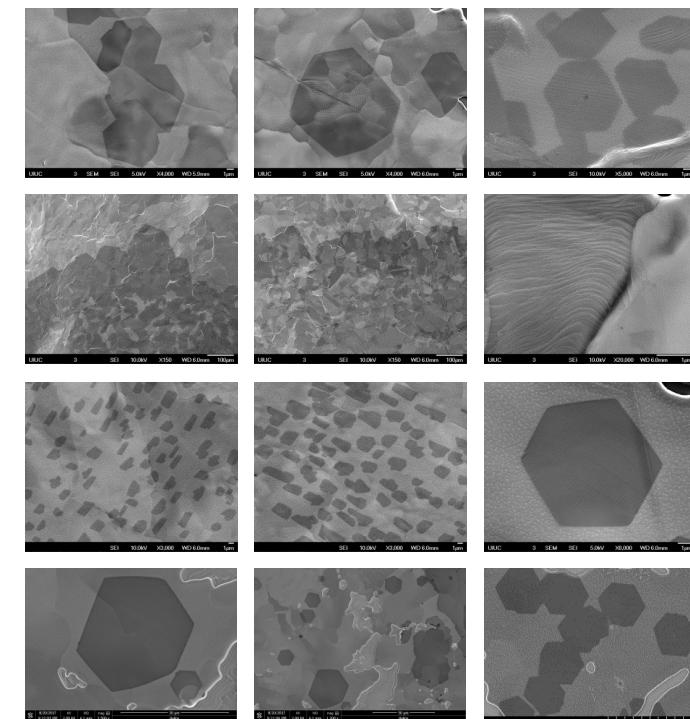
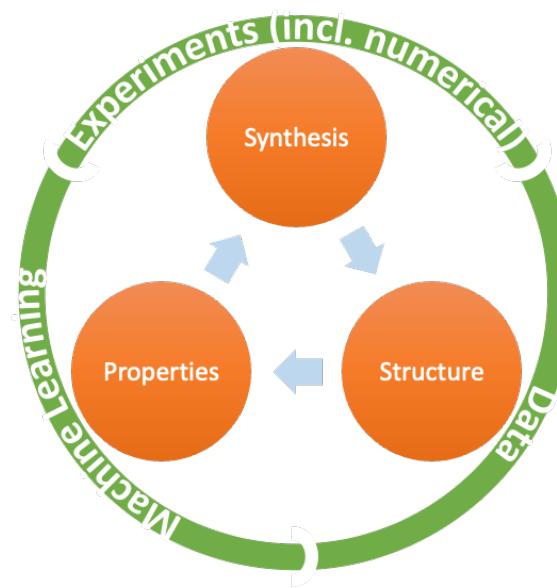
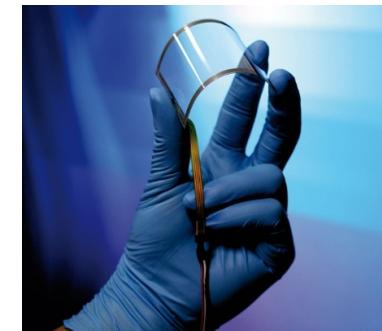
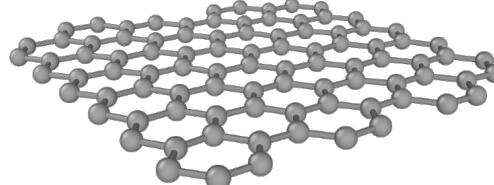
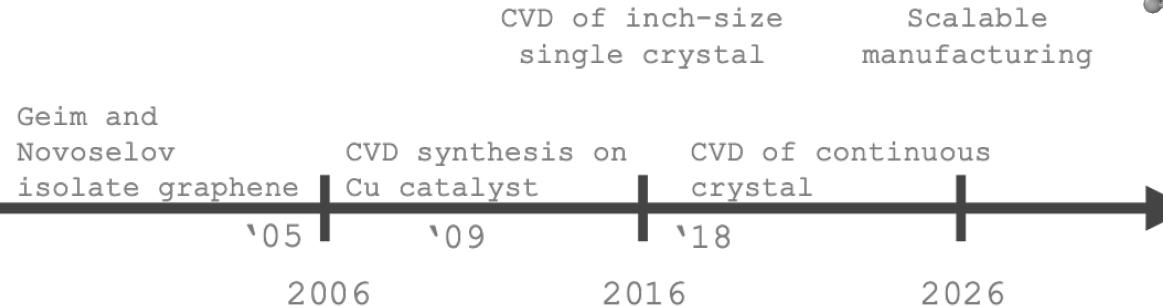
CVD Recipes

- Over 200 variables per sample



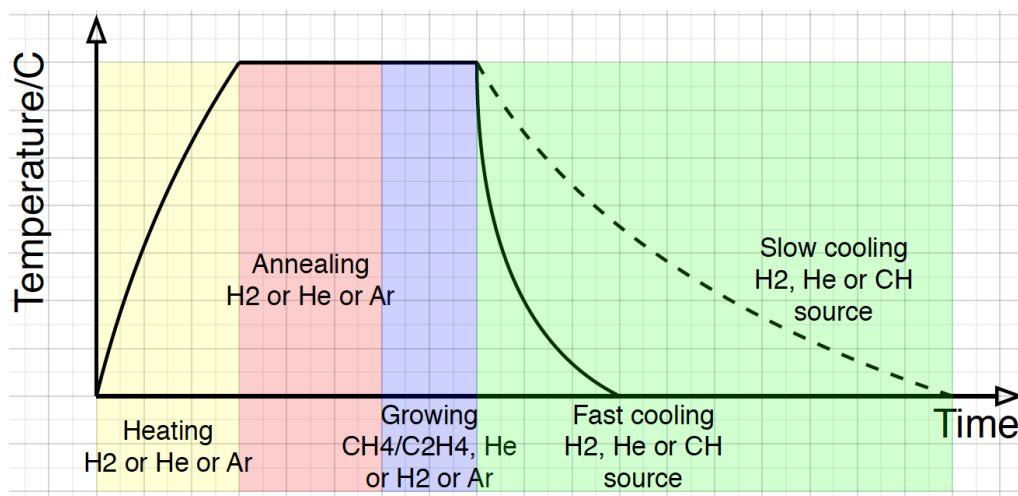
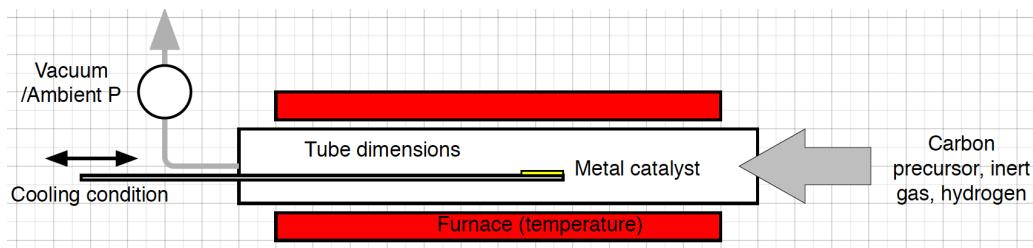
- Furnace temperature
- Furnace pressure
- Gas flow
- Sample position
- Annealing condition
- Growing condition
- Cooling condition
- Sample preparation
- Catalyst
- Furnace dimensions

Lab-scale graphene R&D

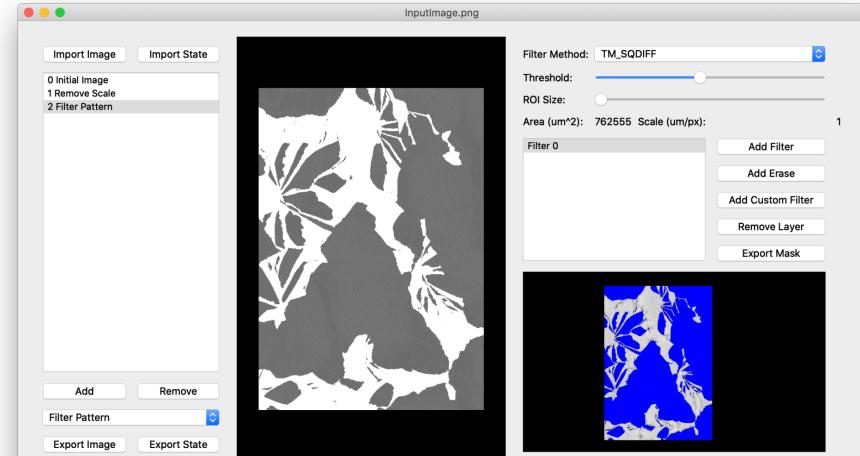
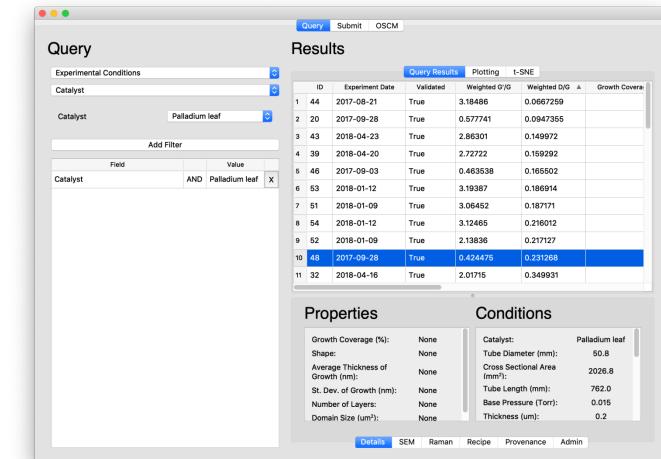
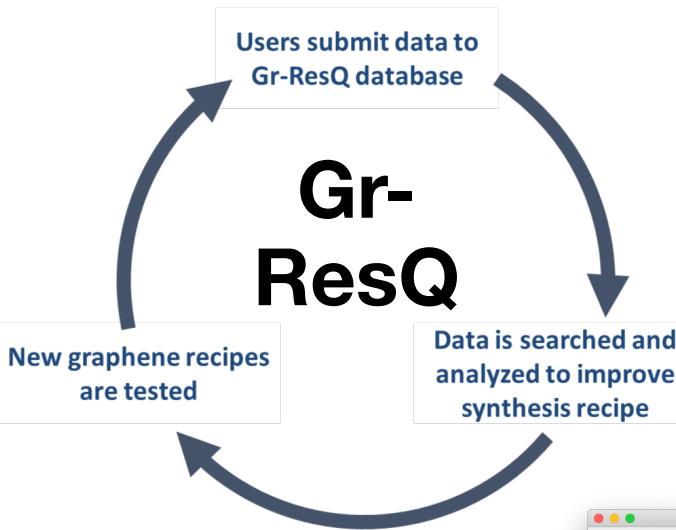
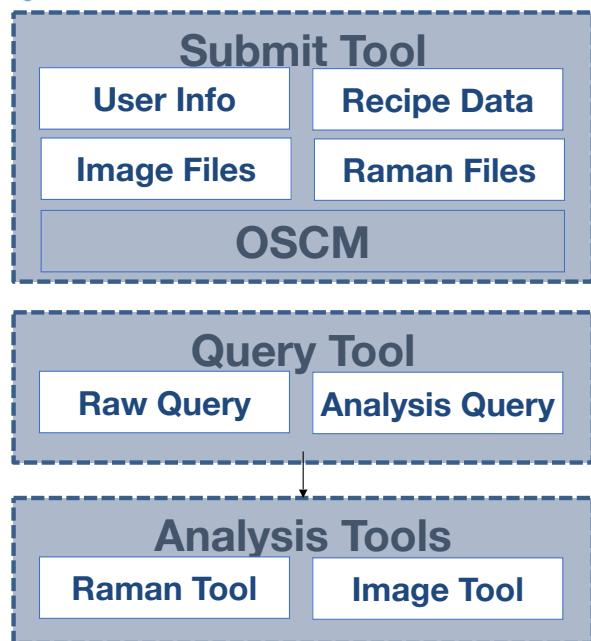
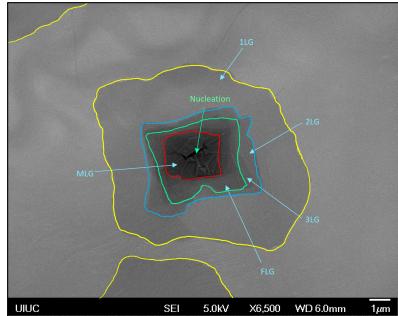


Manufacturability requires cost effectiveness, sustainability, repeatability, etc.

Closed Loop Modeling/ Experimental Optimization of Synthesis

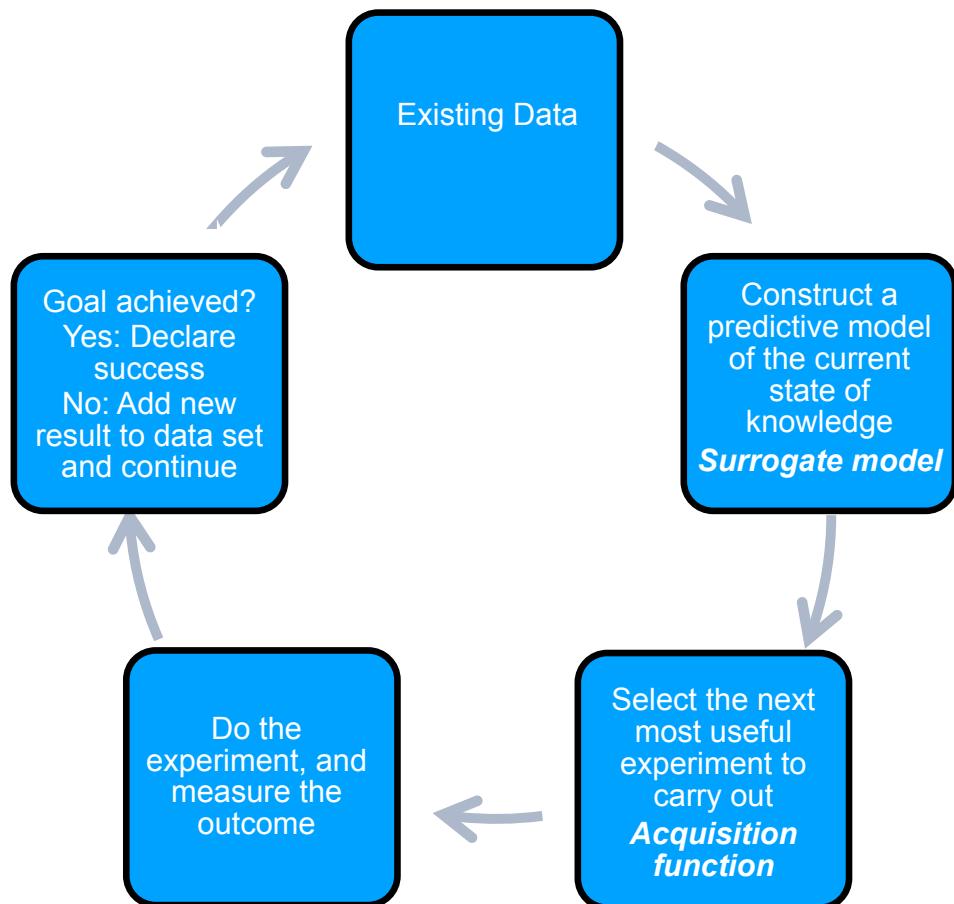


Graphene - Recipes for synthesis of high Quality materials



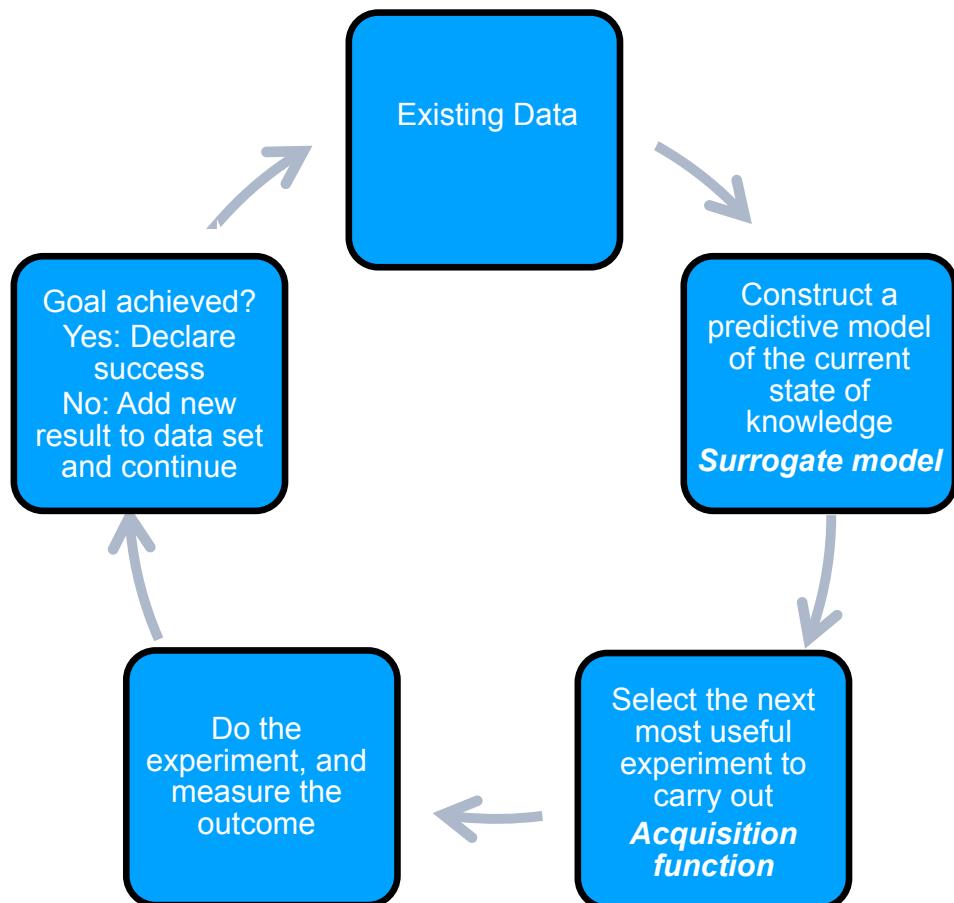
in collaboration with Darren Adams, Placid Ferreira, Sameh Tawfick

Schiller et al., ACS Appl. Nano Mater. 2020, 3, 10, 2020



Closed Loop Modeling/ Experimental Optimization of Synthesis

Bayesian Optimization



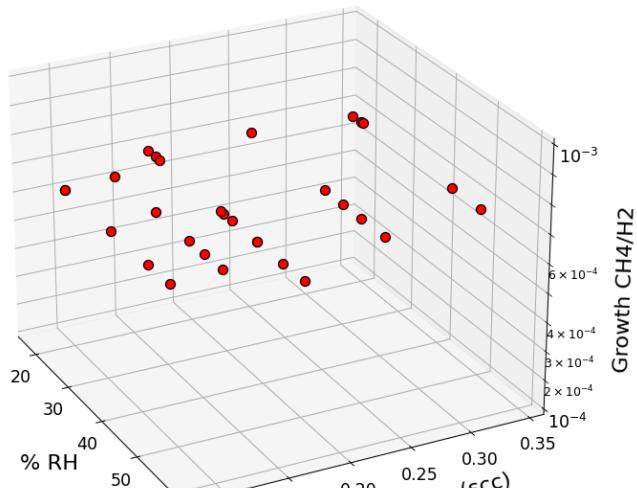
- Design of experiments: initial data set of 20
- Limited set of variable parameters:
 - total CH₄ volume
 - cooling/growth CH₄
 - CH₄/H₂ flow ratio during growth
 - relative humidity
- Synthesis goal: coverage

Bayesian Optimization

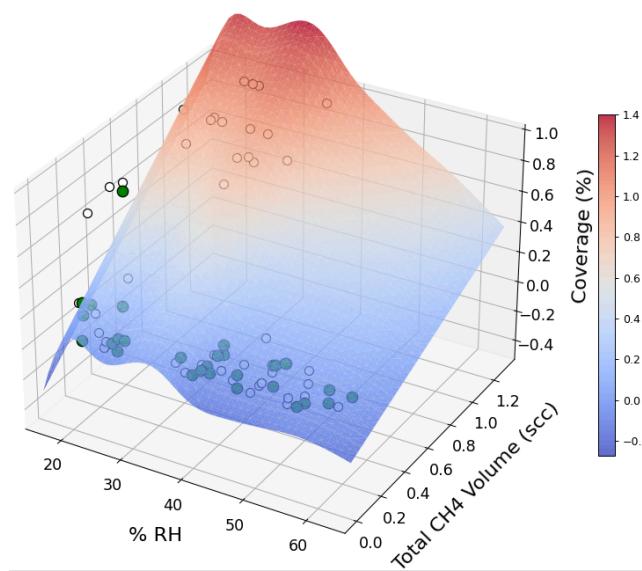


an example cycle:

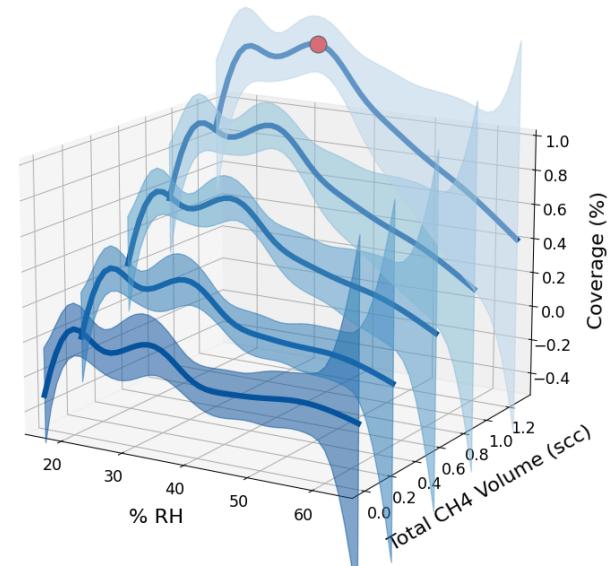
existing data



surrogate model



acquisition function





- Design of experiments: initial data set of 20
- Limited set of variable parameters:
 - total CH₄ volume
 - cooling/growth CH₄
 - CH₄/H₂ flow ratio during growth
 - relative humidity
- Synthesis goal: coverage
- What did we learn? Sweet spot.

