

# NanoMine: Material Informatics for Polymer Nanocomposites ([www.nanomine.org](http://www.nanomine.org))

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Prof. Deborah McGuinness (Rensselaer Polytechnic Institute)



Northwestern  
University



The University of Vermont



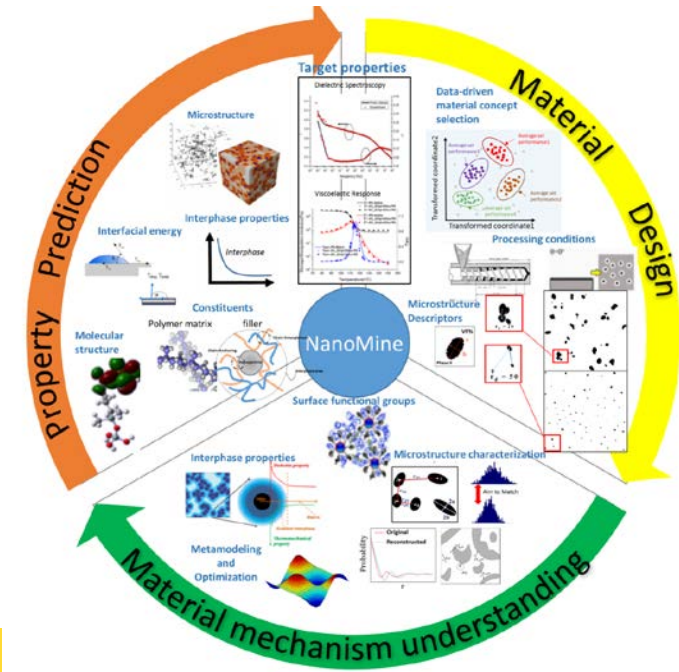
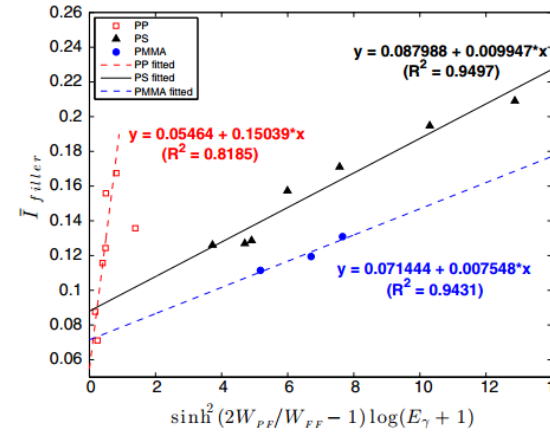
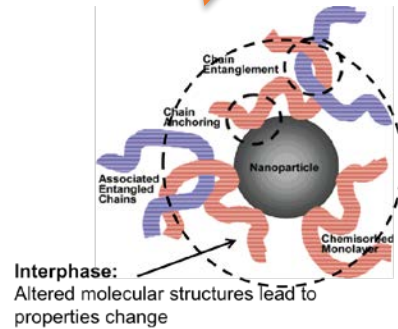
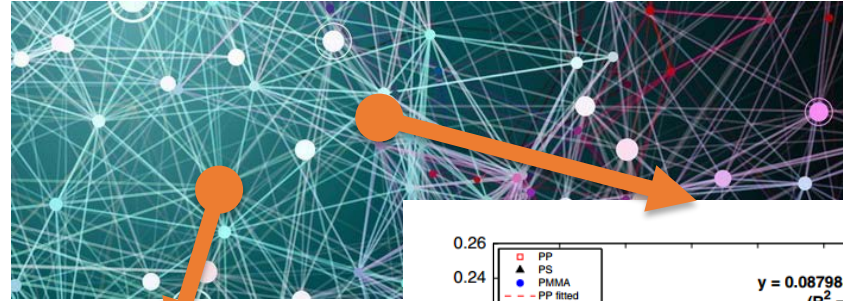
Rensselaer

# Why NanoMine?

Without NanoMine  
 trials and errors



With NanoMine



YES we finally got the papers!

- Then what about
- Data?
  - Plot?
  - Conclusion?
  - Comparison?

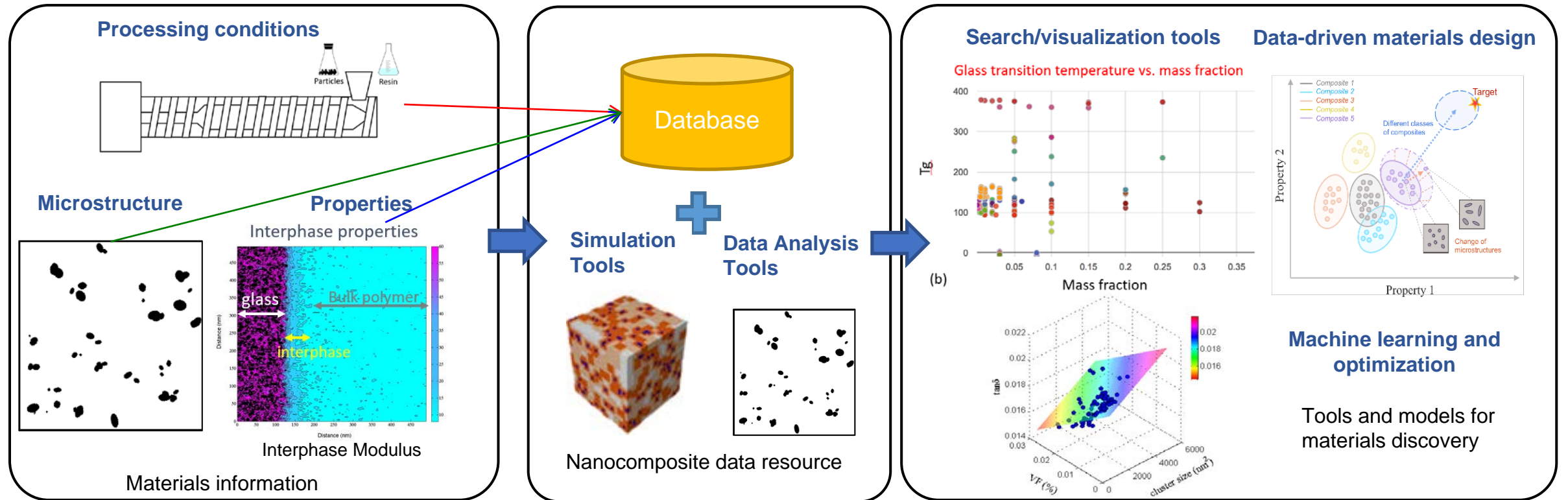


[1] I. Hassinger *et al.*, *J. Mater. Sci.*, vol. 51, no. 9, pp. 4238–4249, 2016.

# What is NanoMine?

**NANO**MINE

NanoMine is an open source, data resource for members of the nanocomposites community.



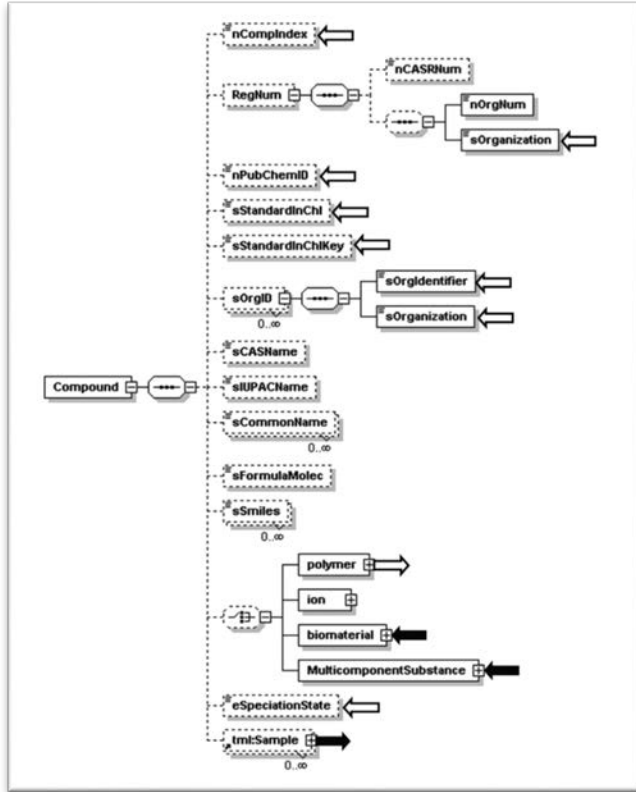
It has **four key goals**:

1. To provide a platform for sharing of data across the community in a format that makes the data findable, accessible, interoperable and reusable (FAIR).
2. To provide a platform for visualizing data, and a mechanism for methods for visualization to be shared.
3. To provide tools that improve the quantification of nanofiller dispersion and morphology as well as the ability to reconstruct those morphologies for subsequent modeling and analysis.
4. To improve the ability to design nanocomposites through simulation and design tools.

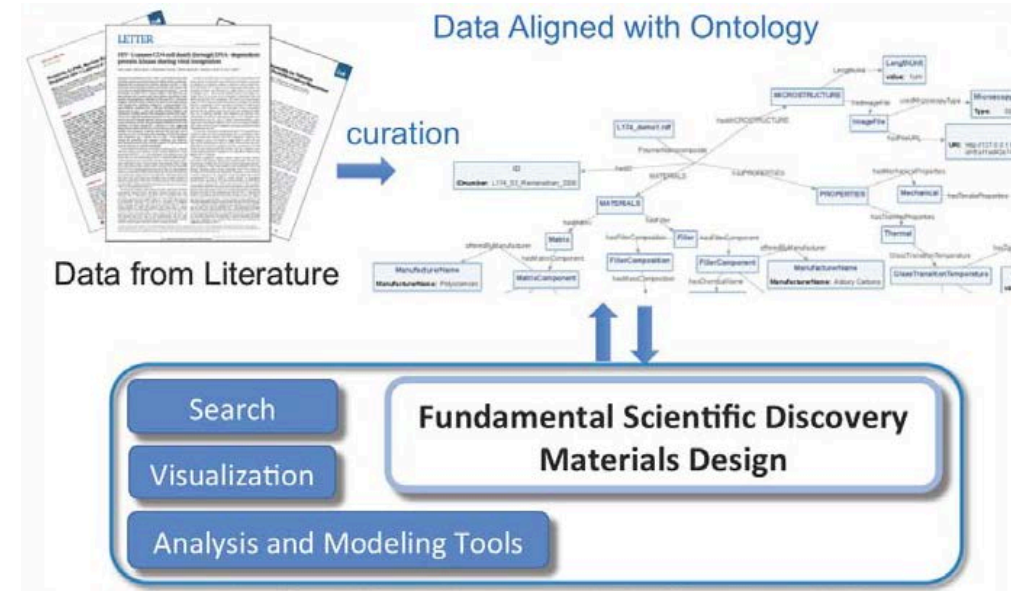
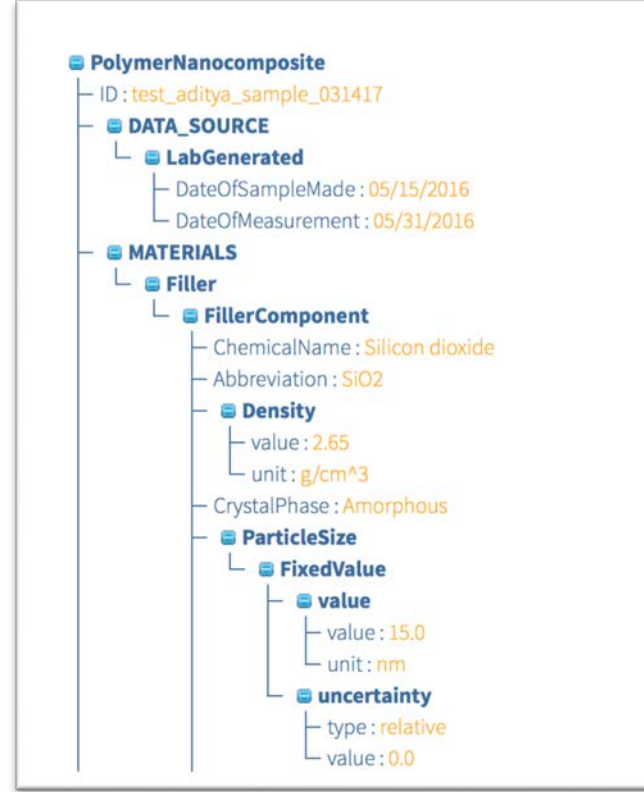
# Database Schema, Structure, and Ontology

NanoMine is built on both a schema and an ontology to provide a robustness to the FAIR principles.

XML Schema



XML/JSON Document



- **200+ entry fields** covering processing, structure and properties
- **200+ set** (papers or lab generated experimental data)
- **1200+ distinctive samples**
- **55 types of polymers**
- **32 types of nanoparticles**

Zhao, H., Li, X., Zhang, Y., Schadler, L. S., Chen, W., & Brinson, L. C. (2016). Perspective: NanoMine: A material genome approach for polymer nanocomposites analysis and design. *APL Materials*, 4(5), 053204.

Zhao, H., Wang, Y., Lin, A., Hu, B., Yan, R., McCusker, J., Chen, W., McGuinness, D. L., Schadler, L. S., & Brinson, L. C. (2018). NanoMine Schema: An Extensible Data Representation for Polymer Nanocomposites. *APL Materials*, accepted.

# Data Curation

## Data Entry

Here you can fill in the Material Data form. Once it is completed, you can view the data you have entered.

Clear Fields Save Form Download

PolymerNanocomposite

SID Sample ID: SIDxxxx

DATA\_SOURCE

MATERIALS

Polymer

Particle

ParticleSurfaceTreatment

PROCESSING

MEASUREMENT\_EQUIPMENT

PROPERTIES

MICROSTRUCTURE

## Data Uploader

### Description

The simplest method to curate your sample into the database is by uploading an MS Excel spreadsheet. An online web-form is also available for the advanced user ([click here](#)). For each sample, upload a template Excel file using the first uploading box and other supplementary image and raw data files using the second uploading box. The master Excel template contains all possible fields for nanocomposite sample data and therefore many fields will remain blank for your sample. Fill in only the parameters applicable to your sample. Customized templates are available upon request, please contact [the administrator](#).

### Steps

- Step 1: Click [here](#) to download the blank MS Excel template (137 kB). (Click [here](#) to see an example, 263 kB)
- Step 2: Fill in the parameters for all applicable cells in the template Excel file. Prepare the supplementary images and raw data files.
- Step 3: Select the template Excel file in the first uploading box.
- Step 4: Select the supplementary images and other raw data files in the second uploading box (press "Ctrl" or "Command" when selecting multiple files), then click Submit to upload your data.
- Step 5: Wait for the feedback message. Please read the message and follow the instructions if an error message is displayed.

### Note

1. We recommend you to upload your control sample first and remember its sample ID.
2. Upload one sample data at a time (one template Excel file along with supplementary files).
3. Rows or sections followed by a "f" sign in the template Excel file can be duplicated. Copy them into additional rows if needed.
4. Acceptable image file format: JPG, PNG, TIF(F). Indicate the full image file name including the extensions in the corresponding cells in the template Excel file.

### Inputs

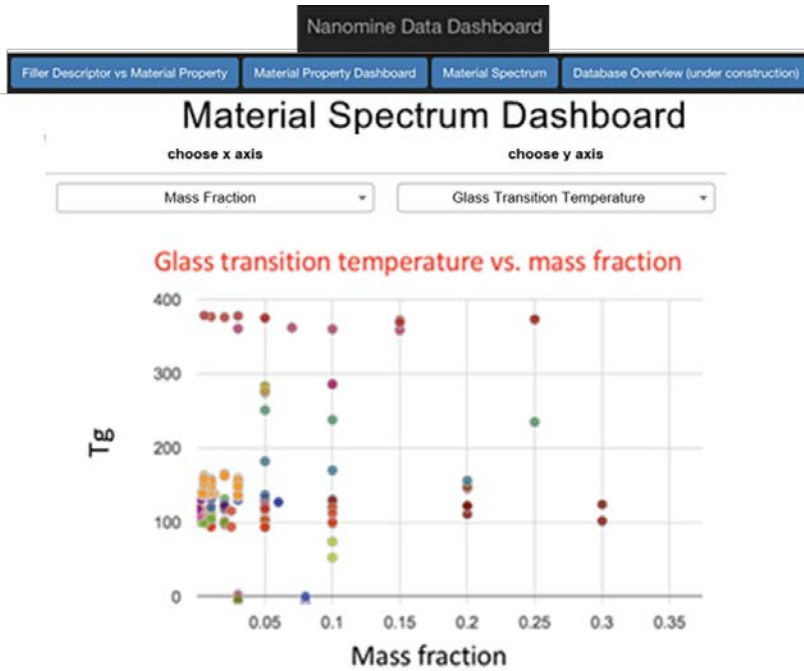
Select the Excel Template File

Select Other Files (including raw data files and image files)

	A	B	C	D	E	F	G	H
1	Polymer							
2								
3	Chemical name							
4	Abbreviation							
5	Polymer class							
6	Polymer type							
7	Manufacture name							
8	Trade name							
9	Density							
10								
11	Particle							
12								
13	Chemical name							
14	Chemical structure							
15	Manufacture name							
16	Particle size							
17	Particle size uncertainty							
18	Specific surface area							
19								

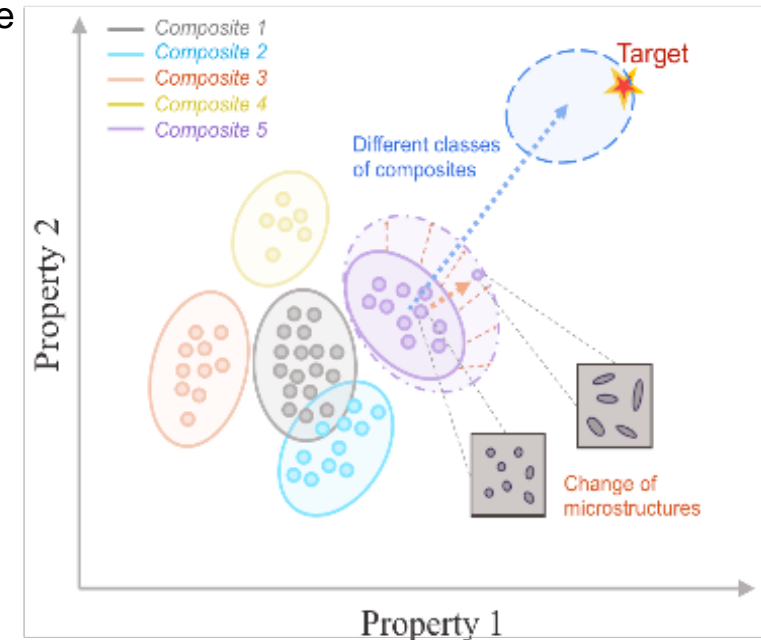
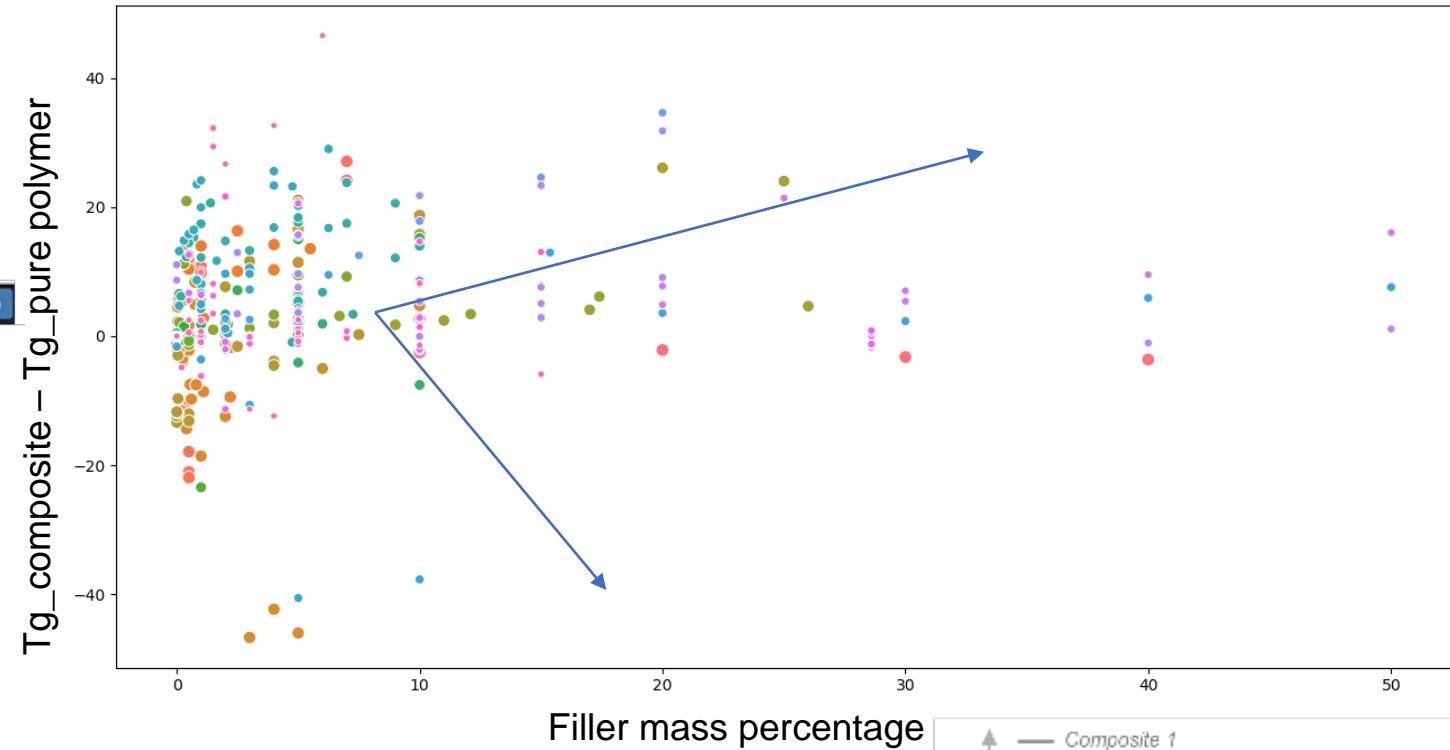
- 1d, 2d, 3d Data types: string/numbers, spectra data, microstructure images
- Two choices of data curation: **Web entry form** and **Excel Template Uploading**
- **Customized Templates** are available!
  - Truncated template based on the research interests of a specific group.
  - Positive feedbacks on the improved efficiency and individual trainings.

# Visualization



- Able to visualize data points in NanoMine
- Able to detect trends among massive amount of data (under development)
- Able to compare personal data with published data (under development)
- Able to inspire material design and material property prediction (under development)

Property comparison against control samples

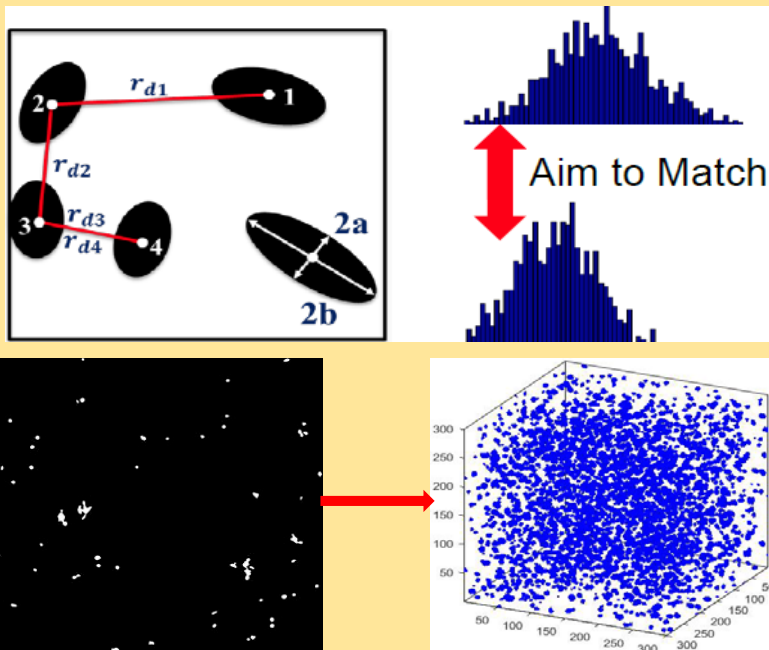


# Microstructure Characterization and Reconstruction (MCR)

**Objective:** Stochastically characterize and subsequently reconstruct the microstructure to enable automation of material design

## Physical Descriptors<sup>2</sup>

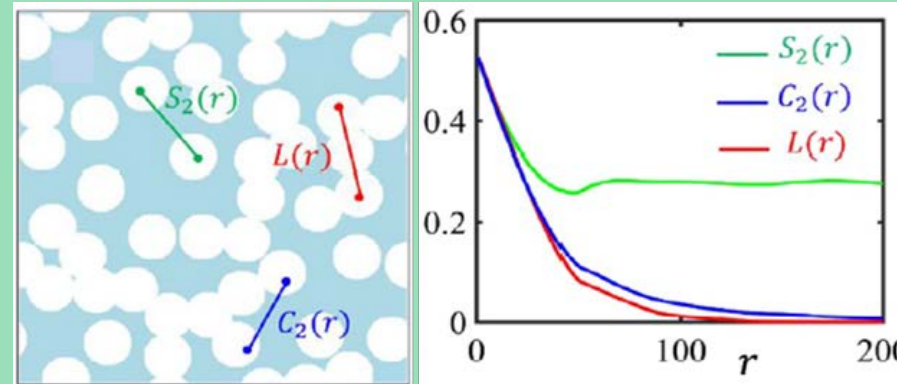
- Characterization via important structural parameters
- Reconstruction via hierarchical optimization



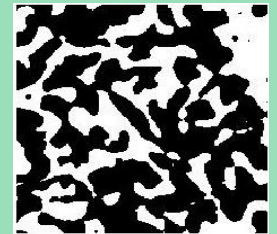
[2] Xu, H. et. al. (2014) J Mech Design, 136, 051007.

## Statistical Functions<sup>1</sup>

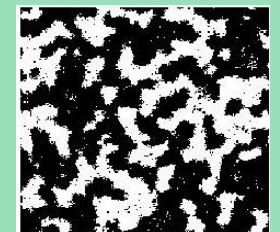
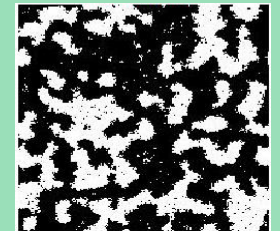
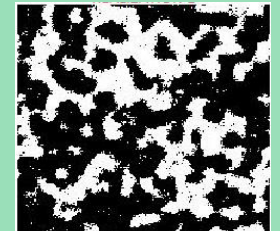
- Spatial correlations characterized in a probabilistic sense:



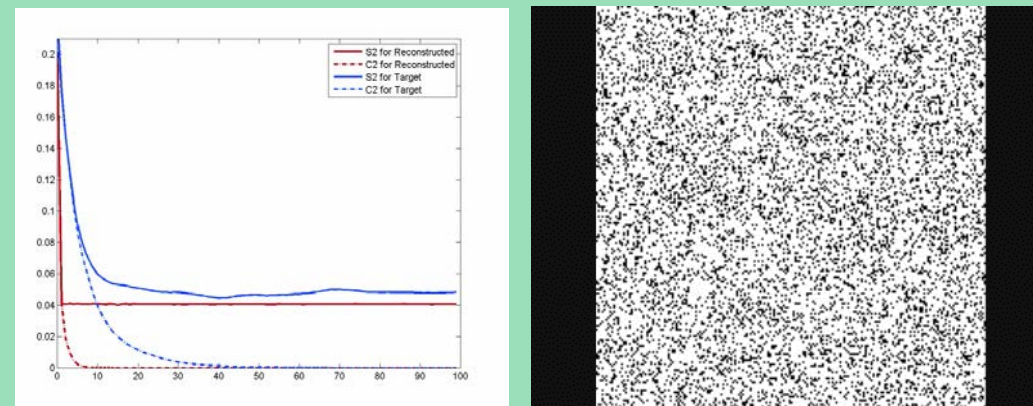
## Target Image



## Statistically Equivalent Reconstructions



- Reconstruction by optimization:

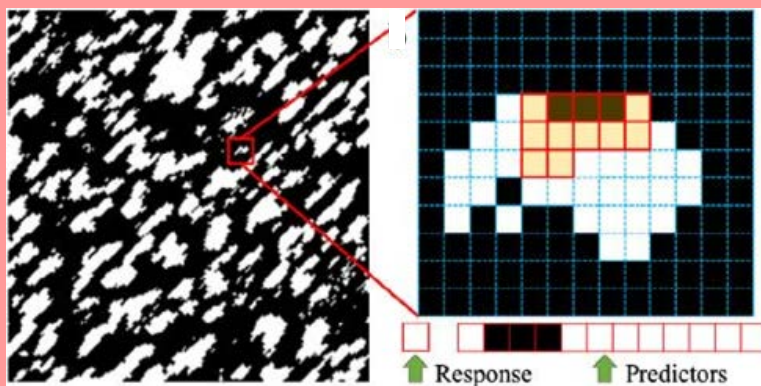


[1] Torquato, S., et al. J Chem Phys 77 (1982) 2071-2077.

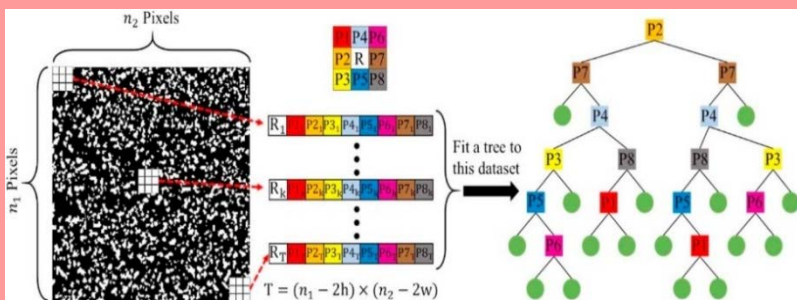
# Microstructure Characterization and Reconstruction(contd.)

## Supervised Learning<sup>3</sup>

- Model phase values as functions of surrounding pixels



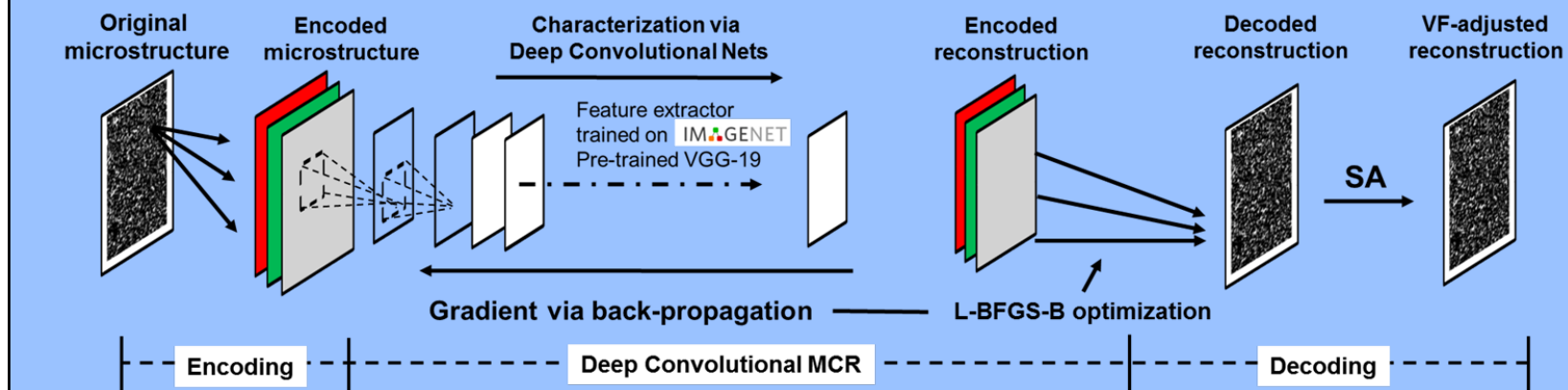
- Decision tree as the supervised learner



[3] Bostanabad, R., et al. (2016) *Acta Materialia*, 103, 89-102.

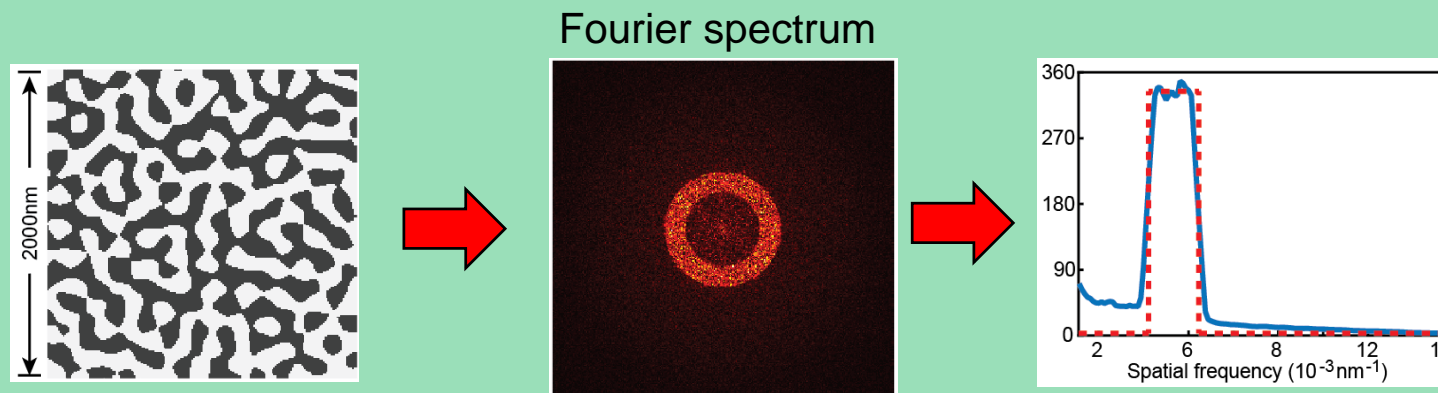
## Deep Convolutional Network<sup>4</sup>

[4] Li, X, et al. (2018)  
Scientific Report, ASME JMD



## Spectral Density Function<sup>5</sup>

- Describes the structural spatial correlations in the frequency domain and enables *physics-aware dimension reduction*.



[5] Yu, S., et al. (2017) *Scientific reports*, 7, 3752.



# MCR Webtools in NanoMine

Input Image

Image Binarized with Niblack's Method

## Image Binarization

- Otsu's Method
- Niblack's Method



## Features:

- All webtools support JPG/TIFF/PNG image formats
- Capable of processing multiple images with a single job request
- Users notified through e-mail after image processing is complete

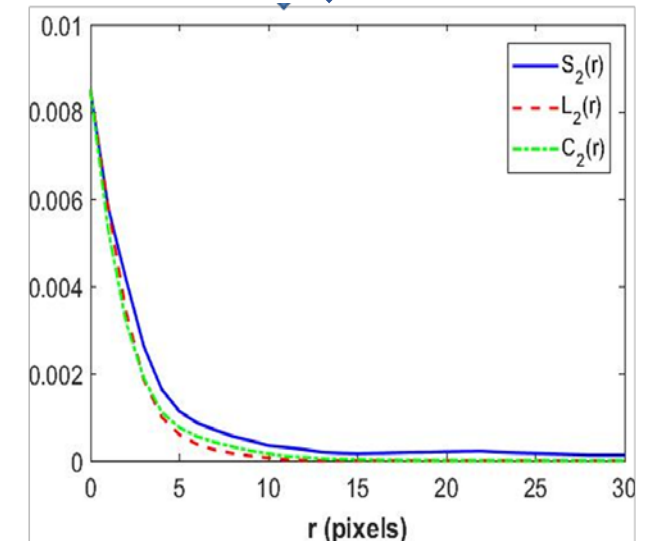
## Microstructure Characterization

- Correlation Functions
- Physical Descriptors
- Spectral Density Function



## Microstructure Reconstruction

- Correlation Functions
- Physical Descriptors
- Spectral Density Function

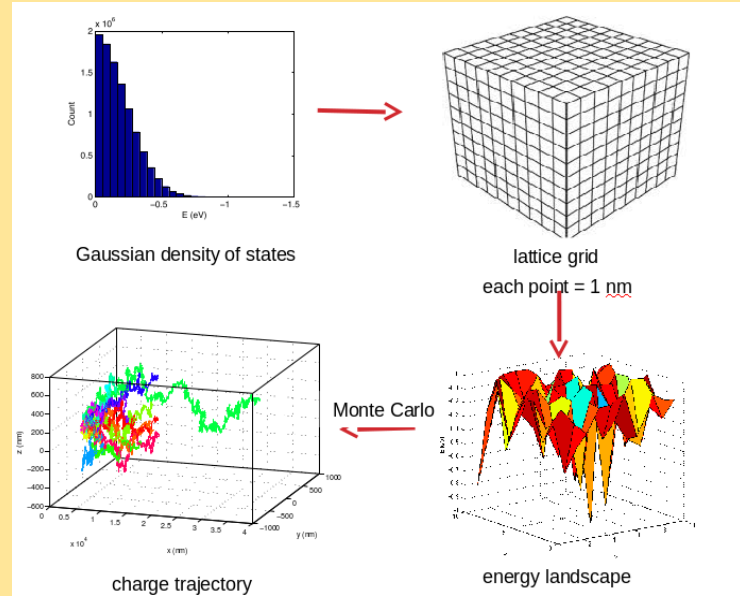


# MCR Webtools in Action



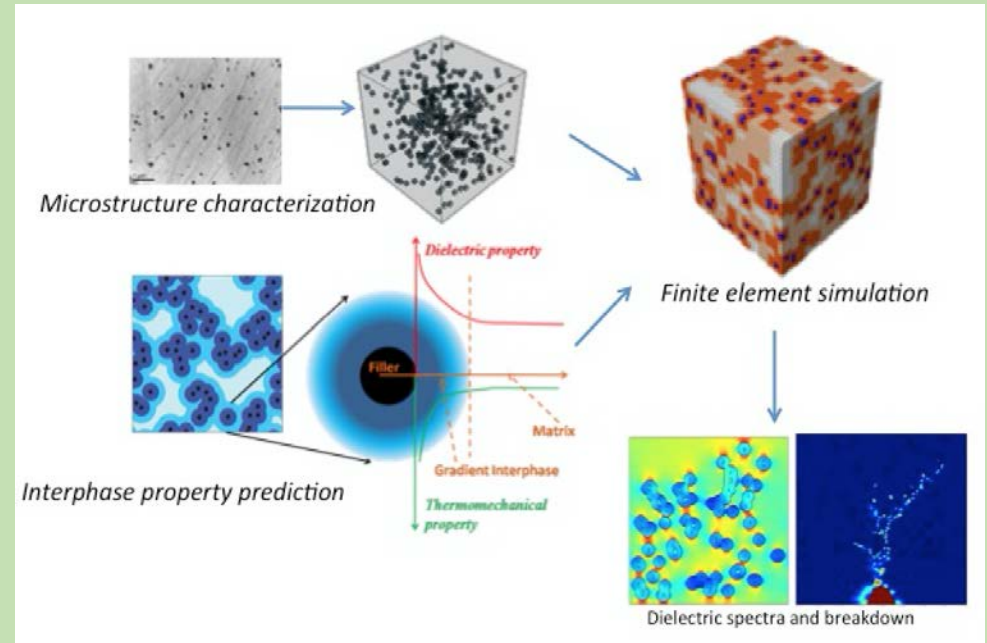
# Material Property Simulation

## Integrated Monte Carlo – Finite Element analysis for Charge Transport simulation<sup>6</sup>

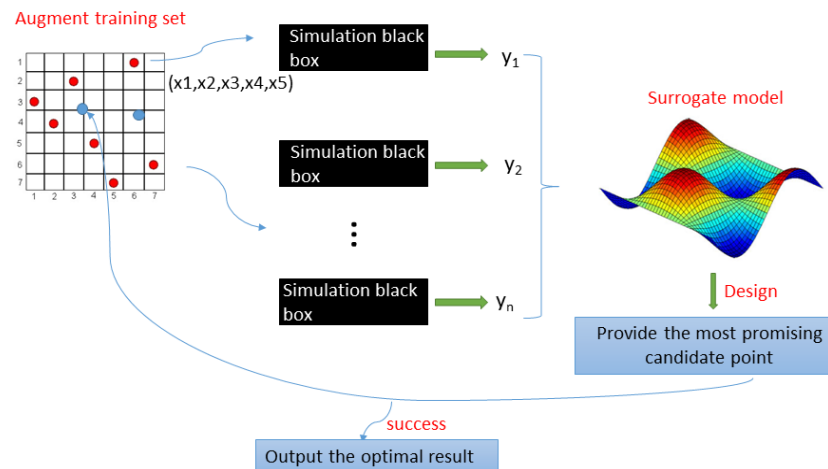


[6] Yanhui Huang, Linda. S. Schadler, arXiv,2016 ([10.1063/1.4945373](https://arxiv.org/abs/10.1063/1.4945373))

## Simulating Dielectric Spectroscopy<sup>7</sup>



[7] Natarajan, Bharath et al., *Macromolecules*, 2013, 46(12)



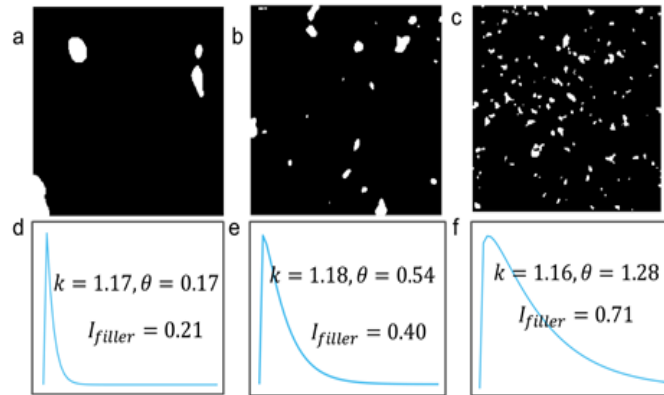
## Automatic fitting of Interphase Relaxation Model<sup>8</sup>

[8] Wang, Y., et al., *Composites Science and Technology*, 2018

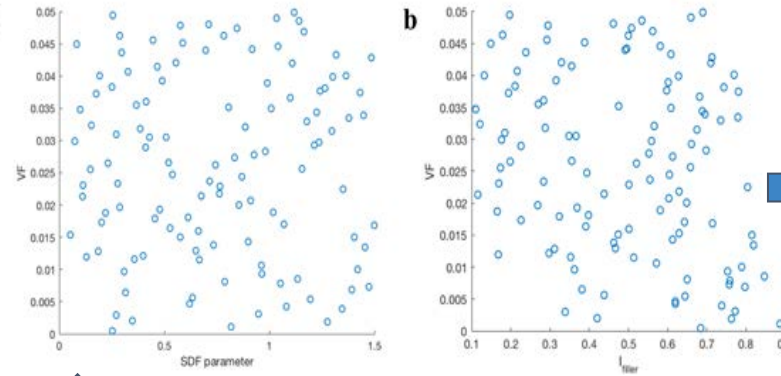
# Case Study: Design of Capacitors

- Objective: Design for high dielectric constant, low dielectric loss materials
  - Material System: PMMA/amino-modified Silica nanocomposites
  - Design Variables: Silica composition, Silica nanoparticle dispersion enabled by Spectral Density Function (SDF)

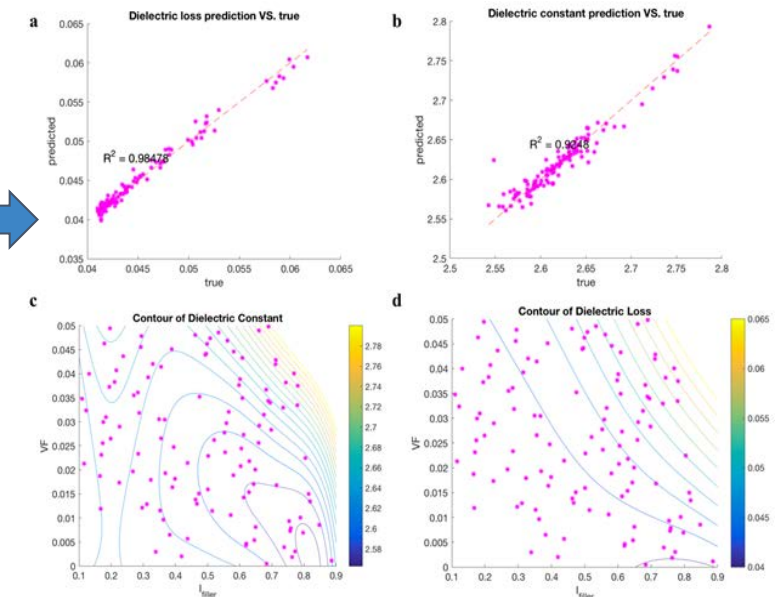
Microstructure Analysis using SDF to determine bounds of Design Variable



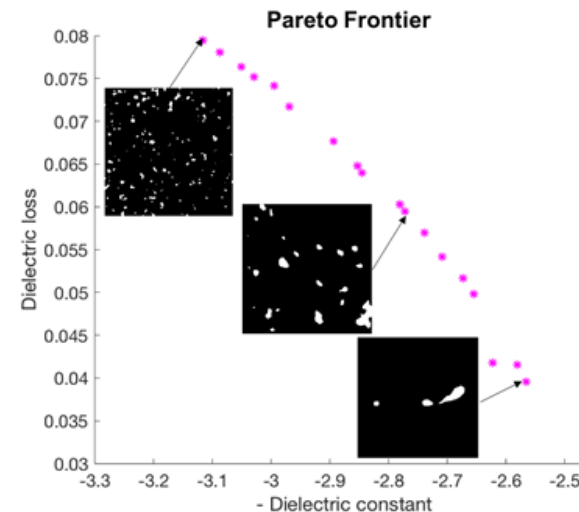
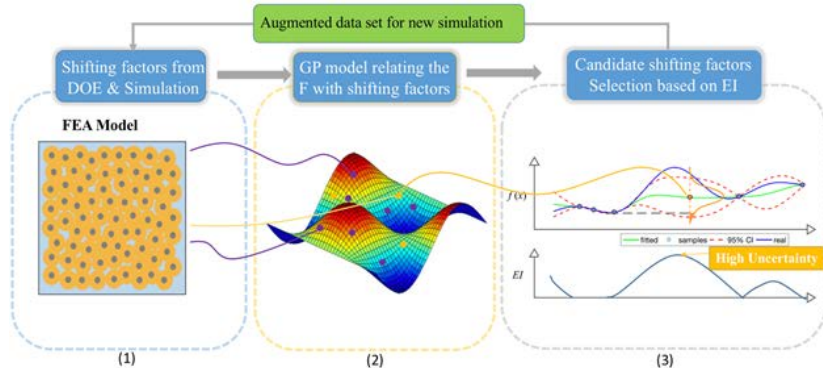
Design of Experiments using Latin Hypercube Sampling to evenly explore design space



Gaussian Process Metamodel created for Dielectric constant and loss prediction to accelerate optimization



Bayesian Optimization to find Interphase shifting parameters



- Multicriteria Genetic Algorithm employed to identify Pareto Frontier
- Structure-Processing mapping used to determine processing conditions to achieve optimal design

# Ongoing and Future Action Items of NanoMine

## **Macromolecules and MacroLetters special Issue: (work in progress)**

- Nearly 20 authors respond to submit; 7 authors have submitted manuscripts
- Online personal trainings on data curation received positive feedbacks

## **Database Development:**

- Authorization: privacy, updates
- Schema Updates

## **Data Curation**

- Predesigned customized templates upon requests
- NLP Assisted Semi-automatic Data Ingestion (for processing info)
  - *Yixing Wang's presentation in MRS session G101.03 on Nov. 27th, 11:30 am, Hynes, Level 1, Room 110*
- Interactive customized templates online (under development)

## **Data Management and Quality Control:**

- Private and Public Data Updates
- Automatic agents assisted data validation throughout and following the curation process

## **Data Visualization:**

- Platform: Visualization Dashboard
- Variety of (innovative) means of Data Visualization: Ashby Plot, etc.

## **NanoMine Enabled Data Analysis and Design**

- Machine learning assisted material property prediction (viscoelastic, dielectric, etc.)
- Addition of Design of Experiments, Metamodeling webtools to facilitate targeted design of materials

# Acknowledgement



# Contacts

- Prof. L Catherine Brinson ([cate.brinson@duke.edu](mailto:cate.brinson@duke.edu) )
- Prof. Wei Chen ([weichen@northwestern.edu](mailto:weichen@northwestern.edu))
- Prof. Linda Schadler ([Linda.Schadler@uvm.edu](mailto:Linda.Schadler@uvm.edu))
- Prof. Deborah L McGuinness ([dlm@cs.rpi.edu](mailto:dlm@cs.rpi.edu))

- Read more about NanoMine:

Zhao, H., Li, X., Zhang, Yi., Schadler L.S., Chen, W., and Brinson, C., "[NanoMine: A Material Genome Approach for Polymer Nanocomposites Analysis and Design](#)", *APL Materials*, **4**, 053204, 2016.