NanoMine: Material Informatics for Polymer Nanocomposites (www.nanomine.org)

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Why NanoMine?

Without NanoMine

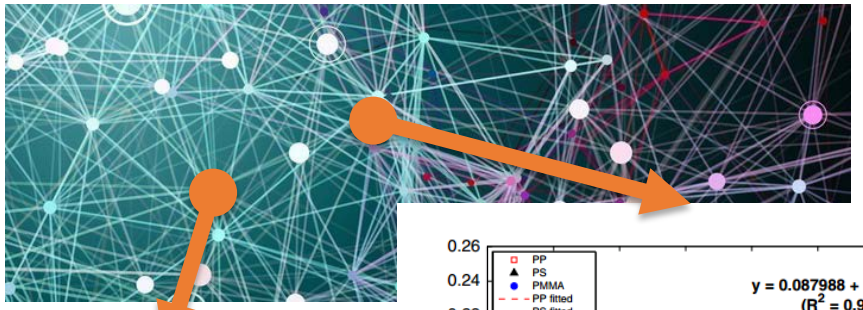
trials and errors

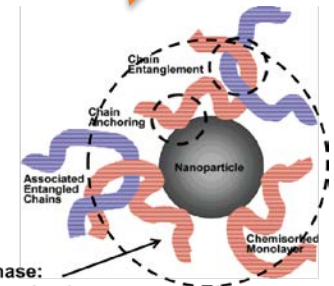
YES we finally got the papers!

Then what about

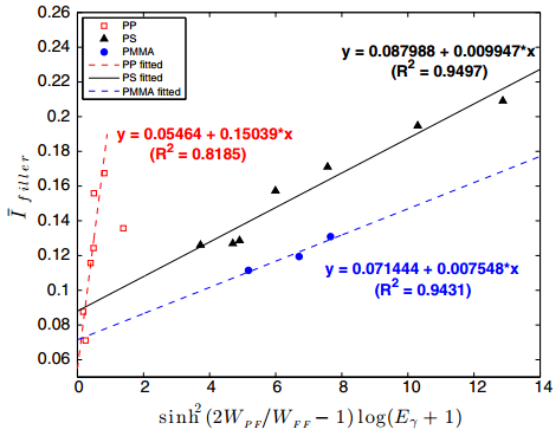
- Data?
- Plot?
- Conclusion?
- Comparison?

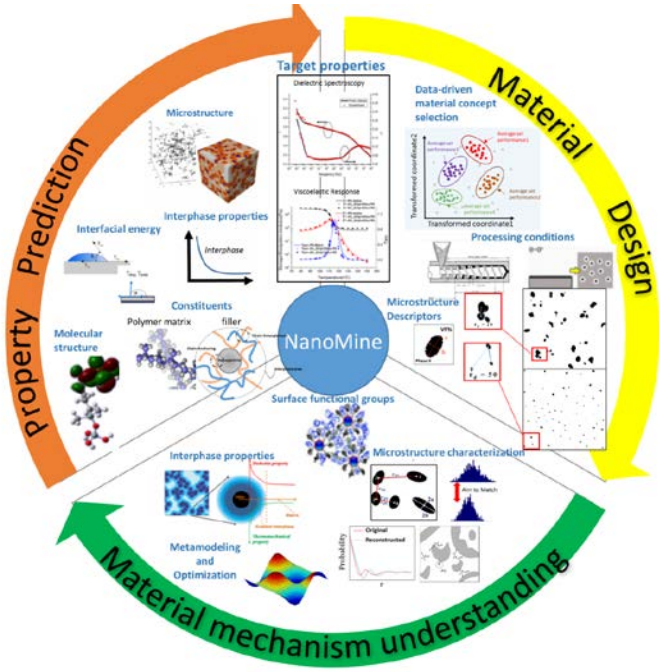
With NanoMine





Interphase:
Altered molecular structures lead to properties change

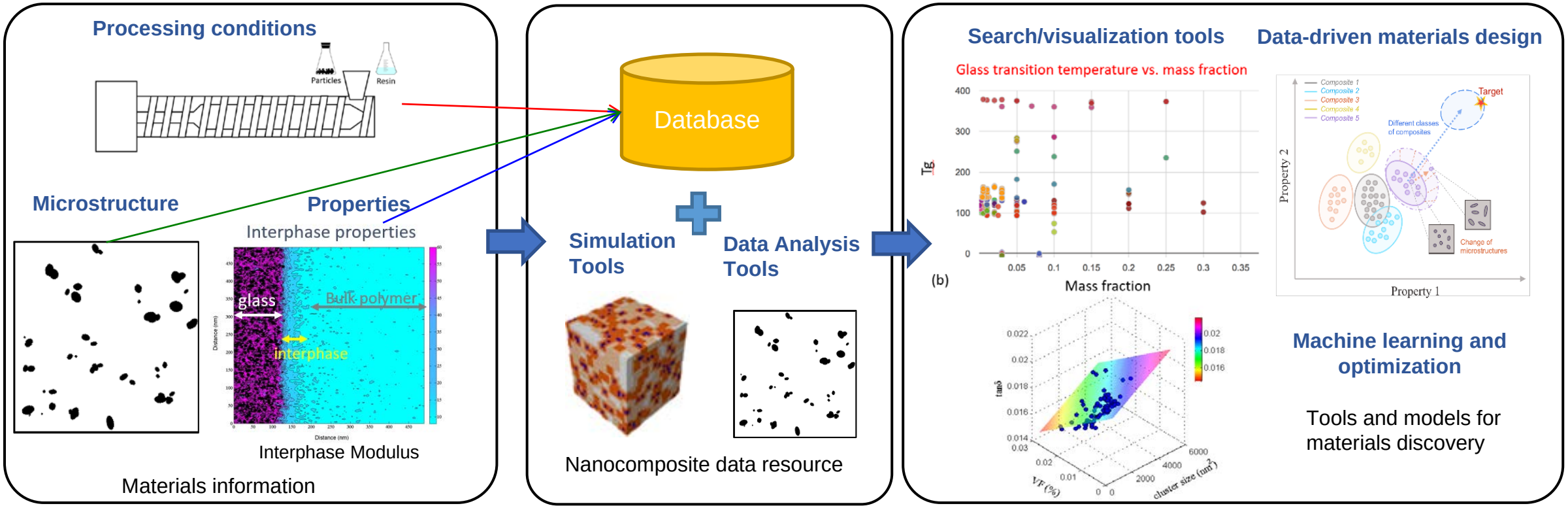




[1] I. Hassinger *et al.*, *J. Mater. Sci.*, vol. 51, no. 9, pp. 4238–4249, 2016.

What is NanoMine?

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



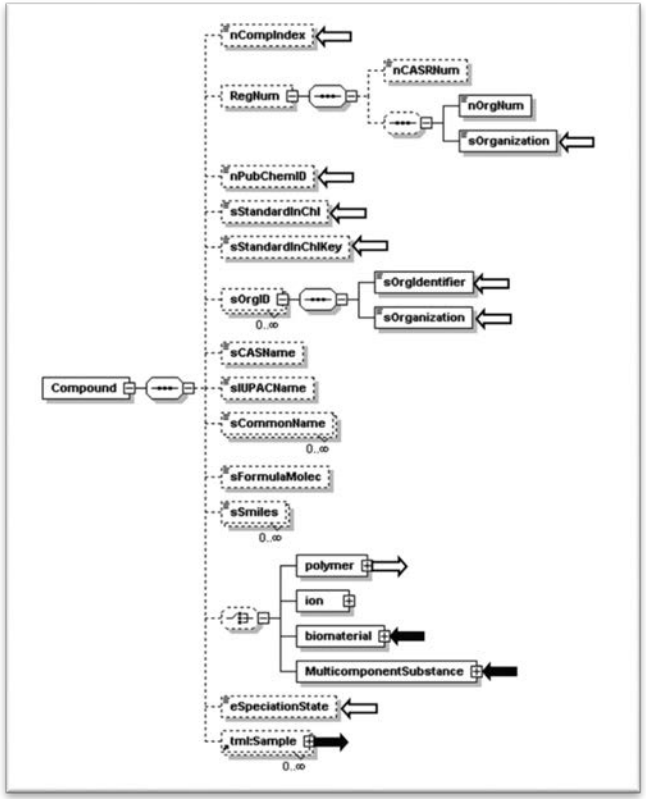
It has **four key goals**:

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.

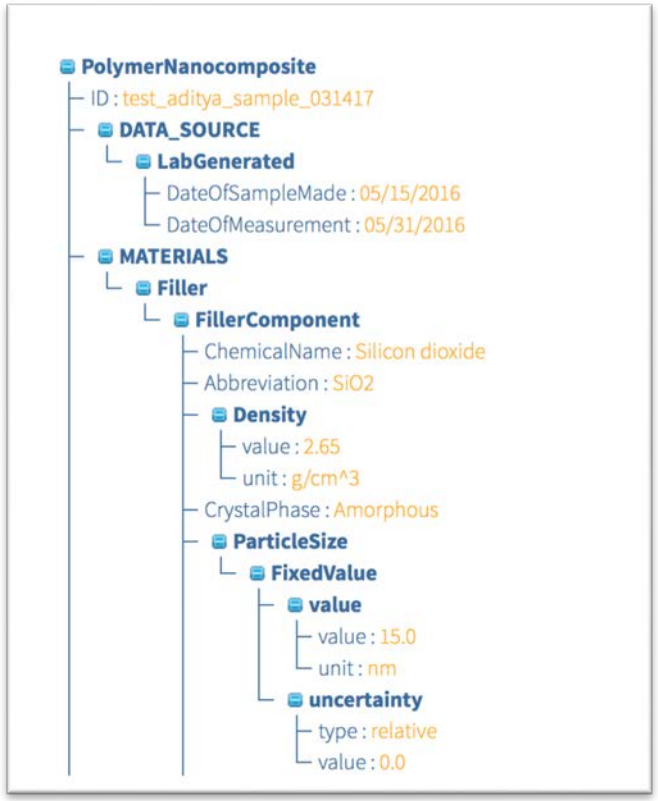
Database Schema, Structure, and Ontology

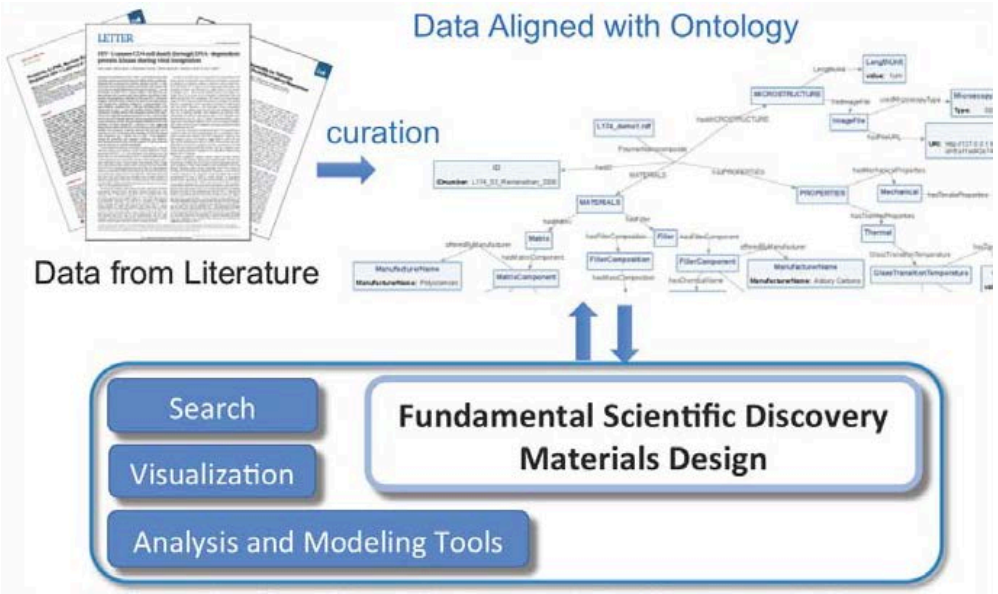
NanoMine is built on both a schema and an ontology to provide a robustness to the FAIR principles.

XML Schema



XML/JSON Document

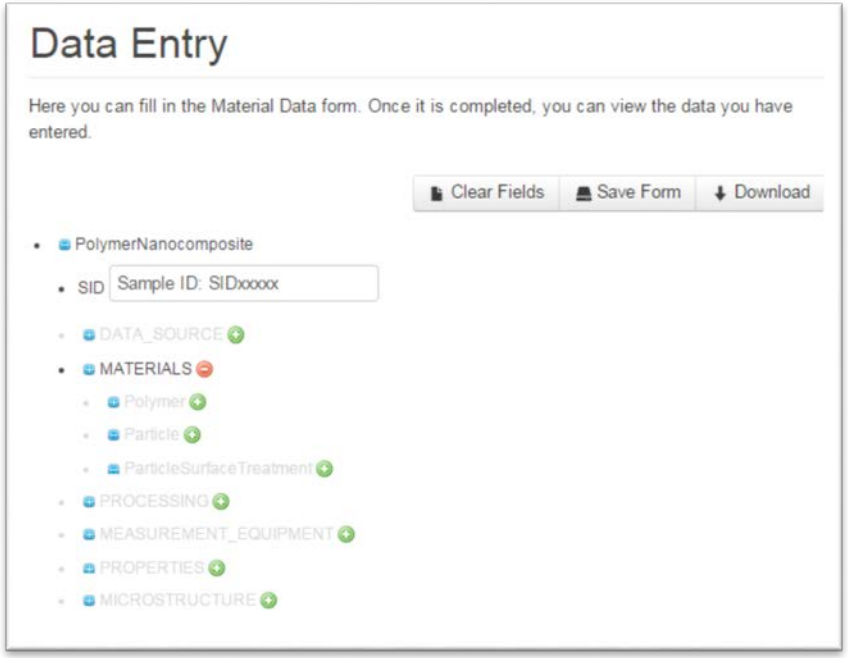


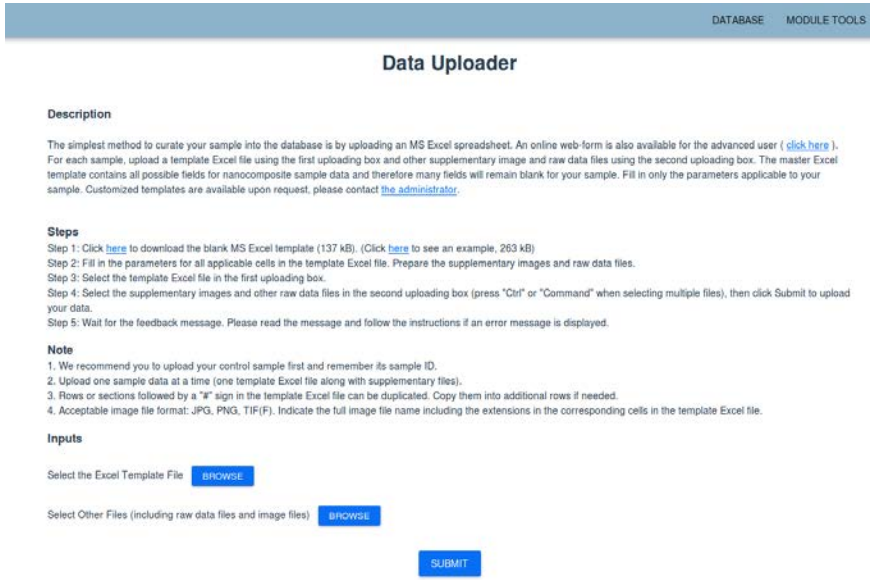


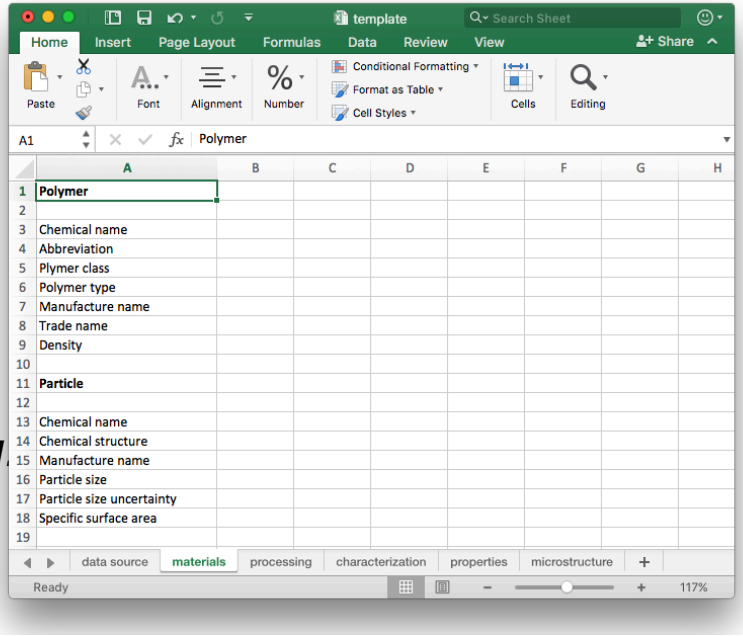
- ***200+ entry fields*** covering processing, structure and properties
- **200+ set** (papers or lab generated experimental data)
- **1200+ distinctive samples**
- **55 types of polymers**
- **32 types of nanoparticles**

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

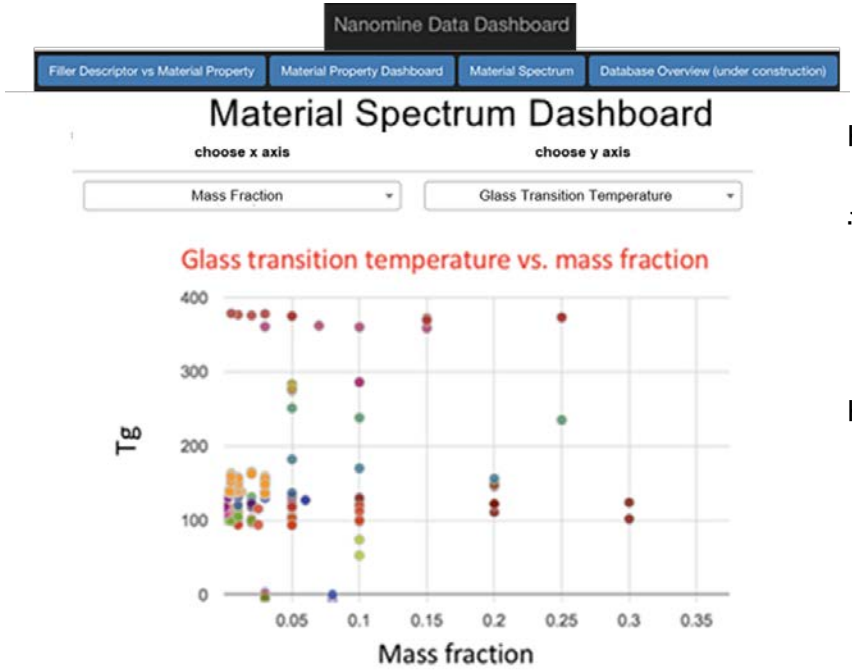


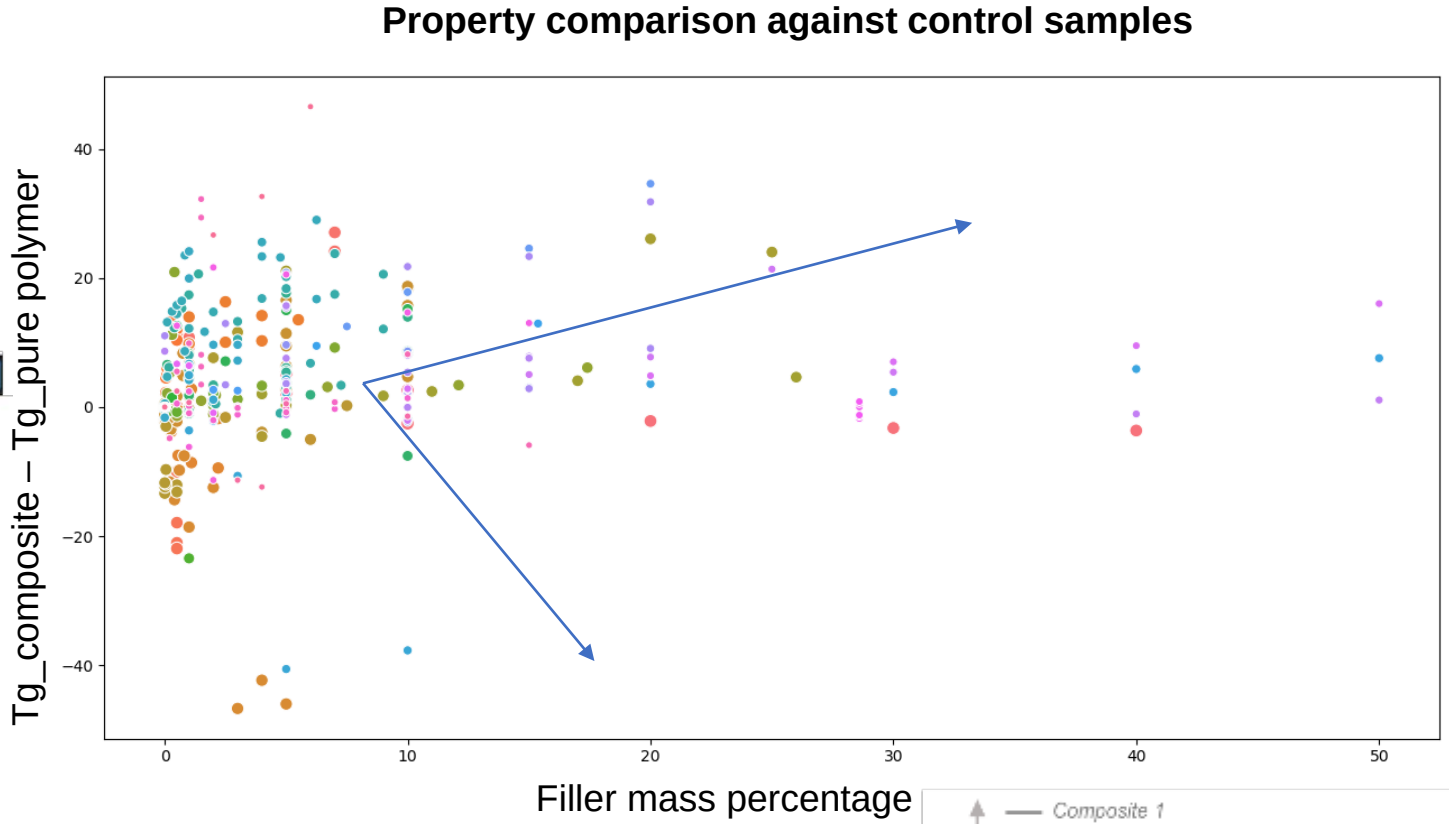


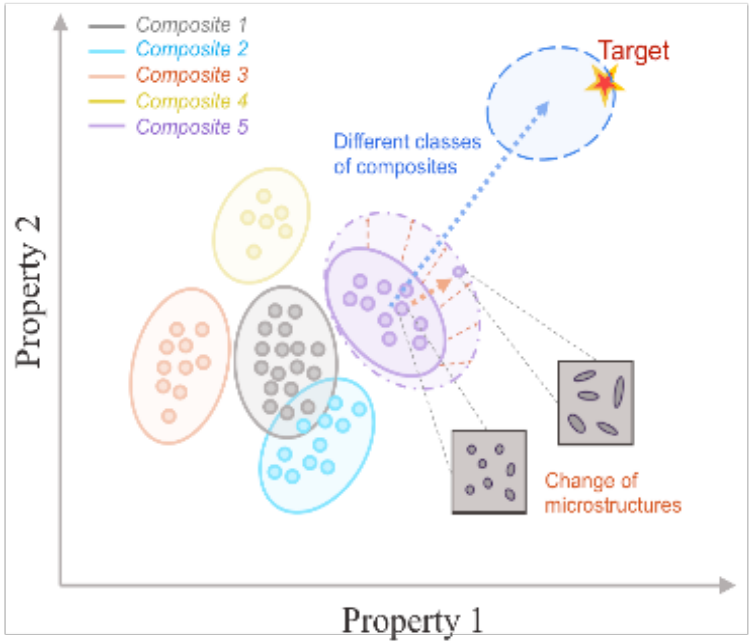


- *1d, 2d, 3d Data types: string/numbers, spectra data, microstructure images*
- *Two choices of data curation: **Web entry form** and **Excel Template Uploading***
- ***Customized Templates** are available!*
  - *Truncated template based on the research interests of a specific group.*
  - *Positive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

Visualization







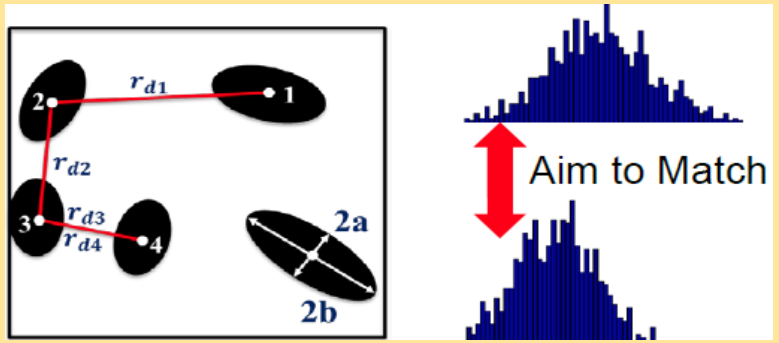
- Able to visualize data points in NanoMine
- Able to detect trends among massive amount of data (under development)
- Able to compare personal data with published data (under development)
- Able to inspire material design and material property prediction (under development)

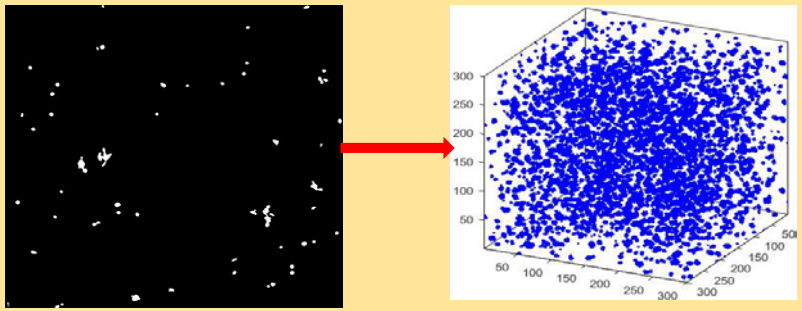
Microstructure Characterization and Reconstruction (MCR)

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

Physical Descriptors[2]

- **Characterization via important structural parameters**
- **Reconstruction via hierarchical optimization**

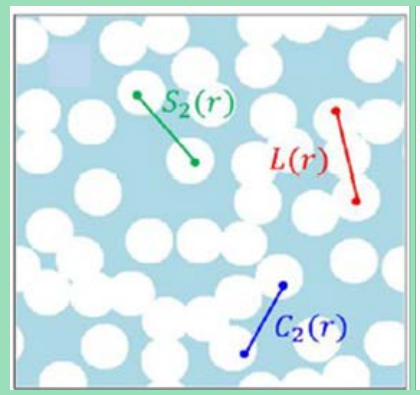


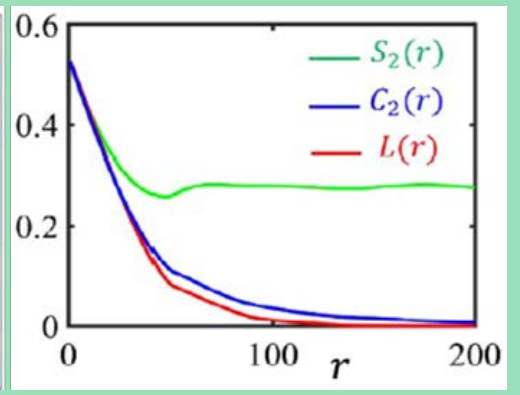


[2] Xu, H. et. al. (2014) J Mech Design, 136, 051007.

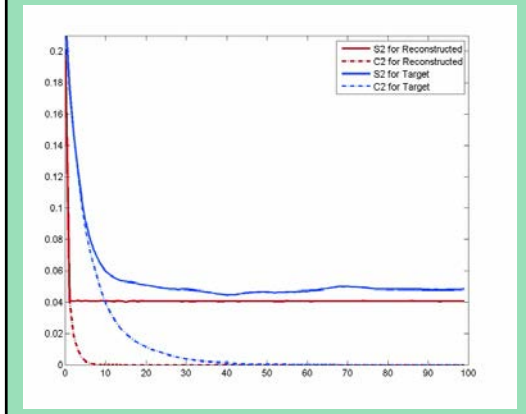
Statistical Functions[1]

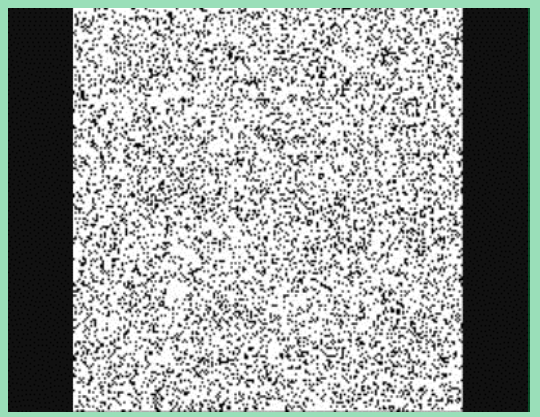
- **Spatial correlations characterized in a probabilistic sense:**



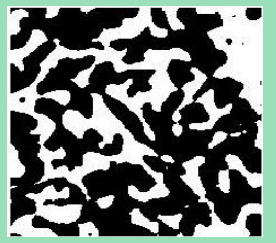


- **Reconstruction by optimization:**

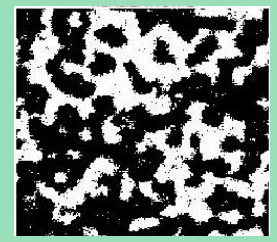


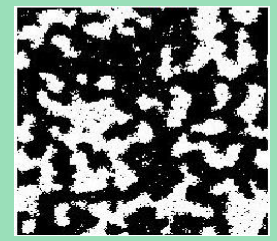


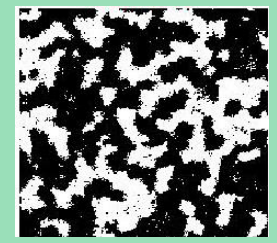
Target Image



Statistically Equivalent Reconstructions





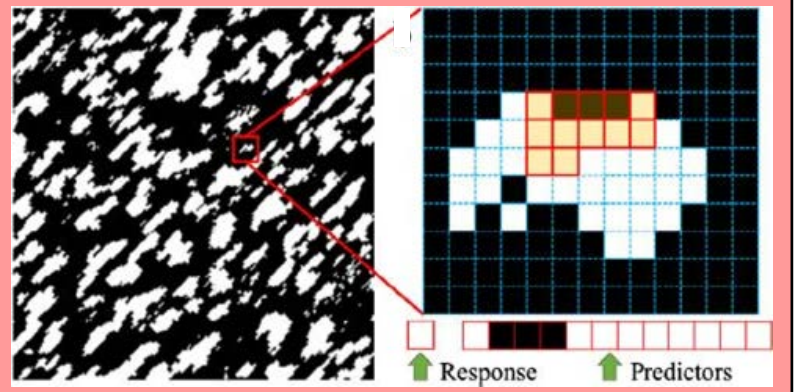


[1] Torquato. S., et al. *J Chen Phys* 77 (1982) 2071-2077.

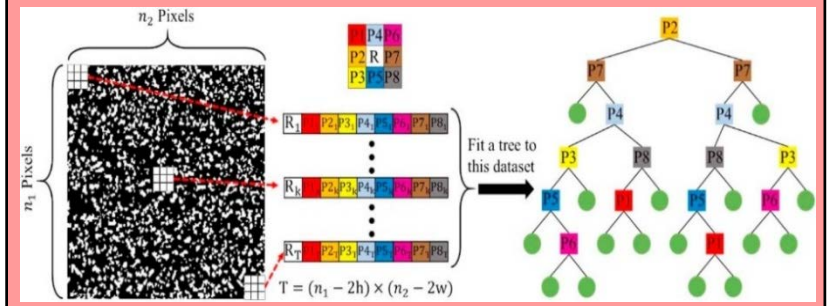
Microstructure Characterization and Reconstruction(contd.)

Supervised Learning[3]

- Model phase values as functions of surrounding pixels



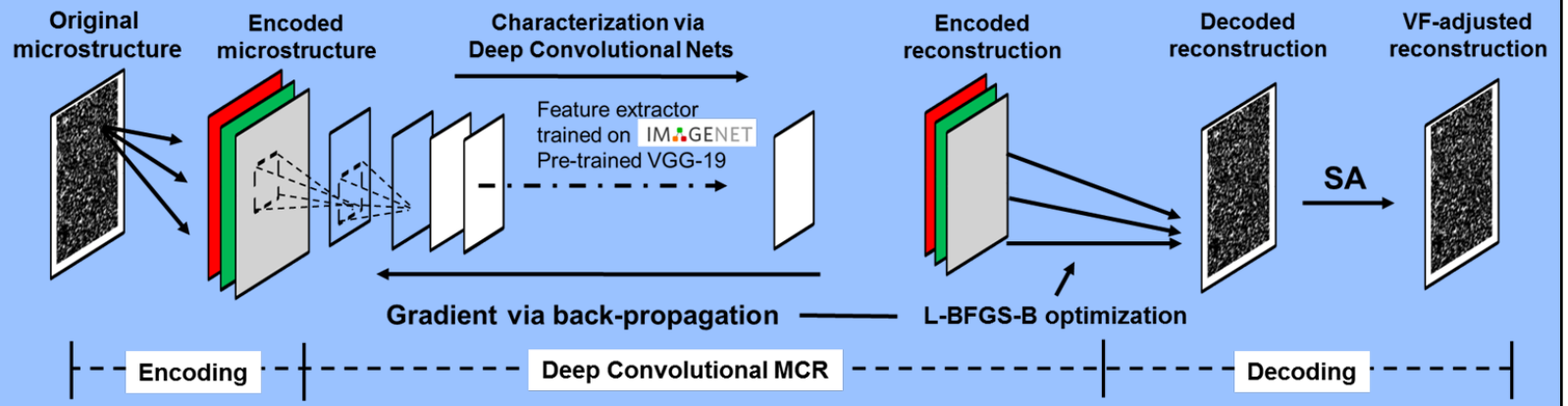
- Decision tree as the supervised learner



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

Deep Convolutional Network[4]

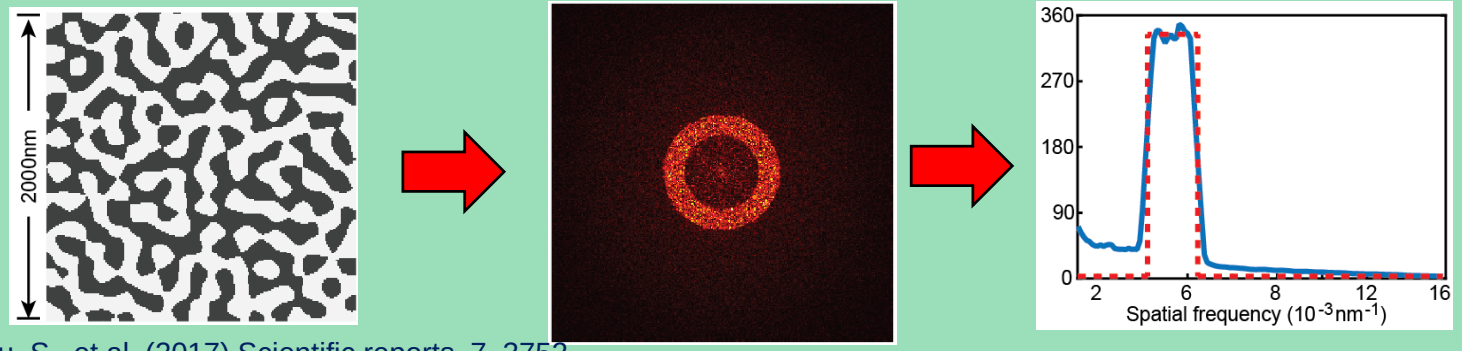
[4] Li, X, et al. (2018) Scientific Report, ASME JMD



Spectral Density Function[5]

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

Fourier spectrum



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

MCR Webtools in NanoMine

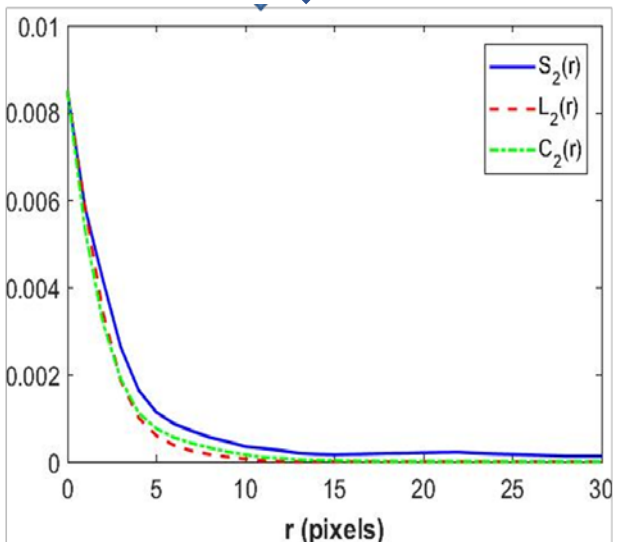
Input Image

Image Binarized with Niblack's Method

Image Binarization
- Otsu's Method
- Niblack's Method

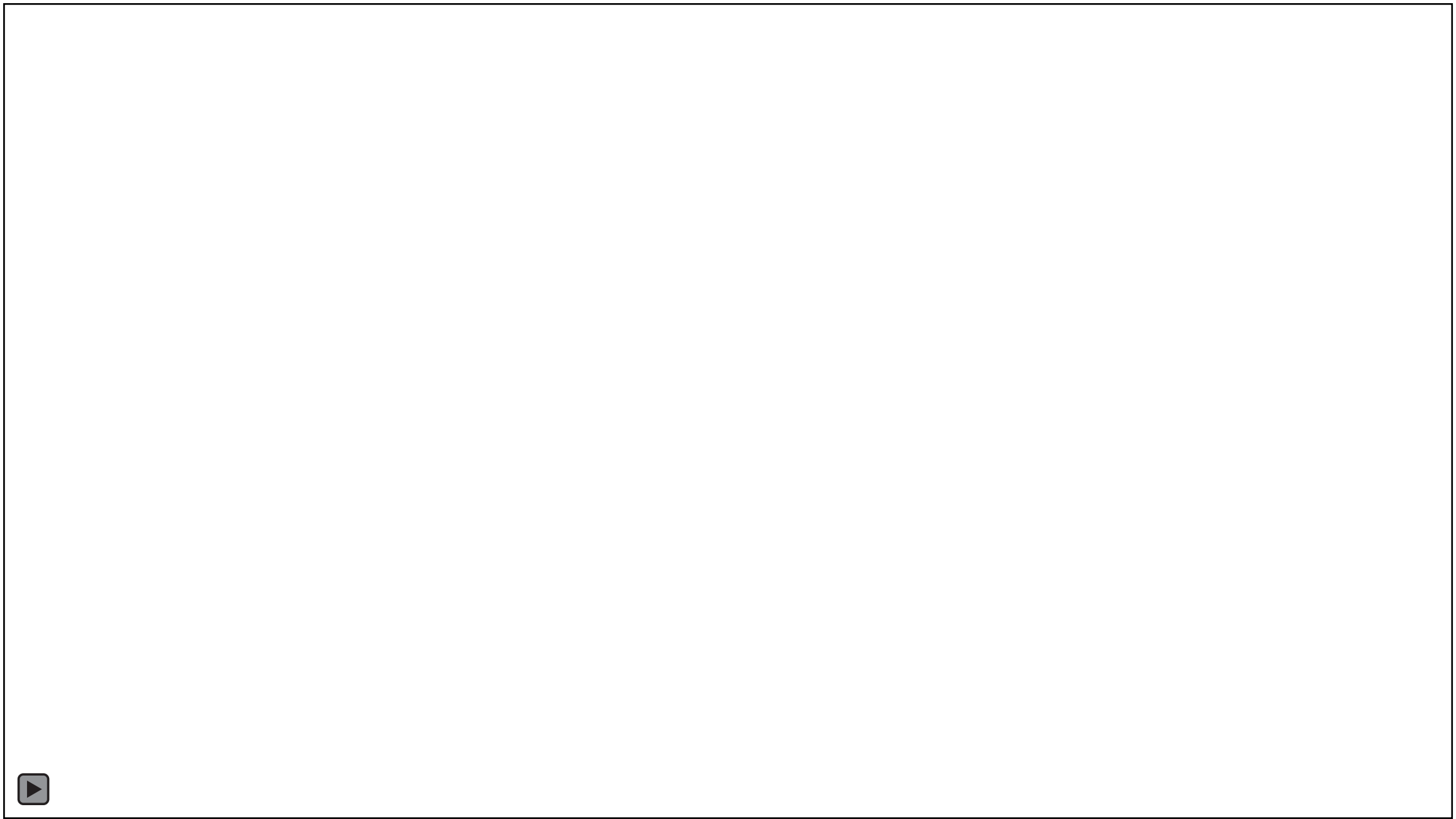
Features:
- All webtools support JPG/TIFF/PNG image formats
- Capable of processing multiple images with a single job request
- Users notified through e-mail after image processing is complete

Microstructure Characterization
- Correlation Functions
- Physical Descriptors
- Spectral Density Function



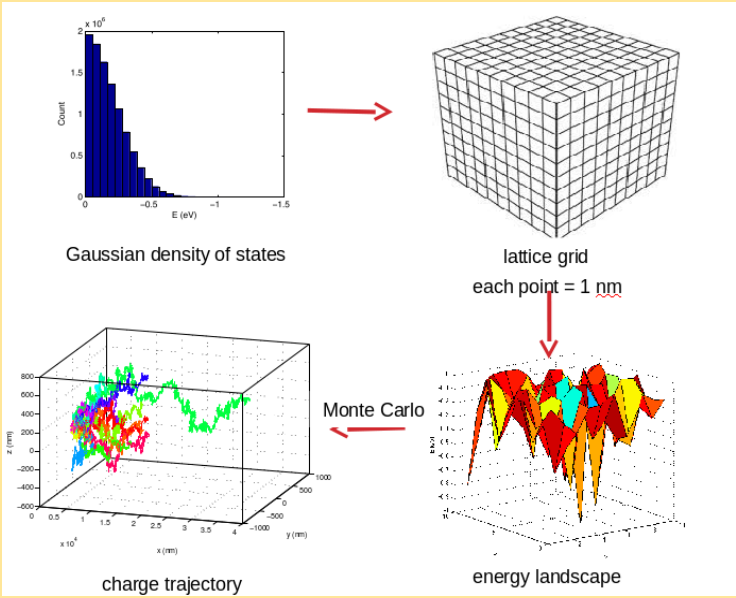
Microstructure Reconstruction
- Correlation Functions
- Physical Descriptors
- Spectral Density Function

MCR Webtools in Action



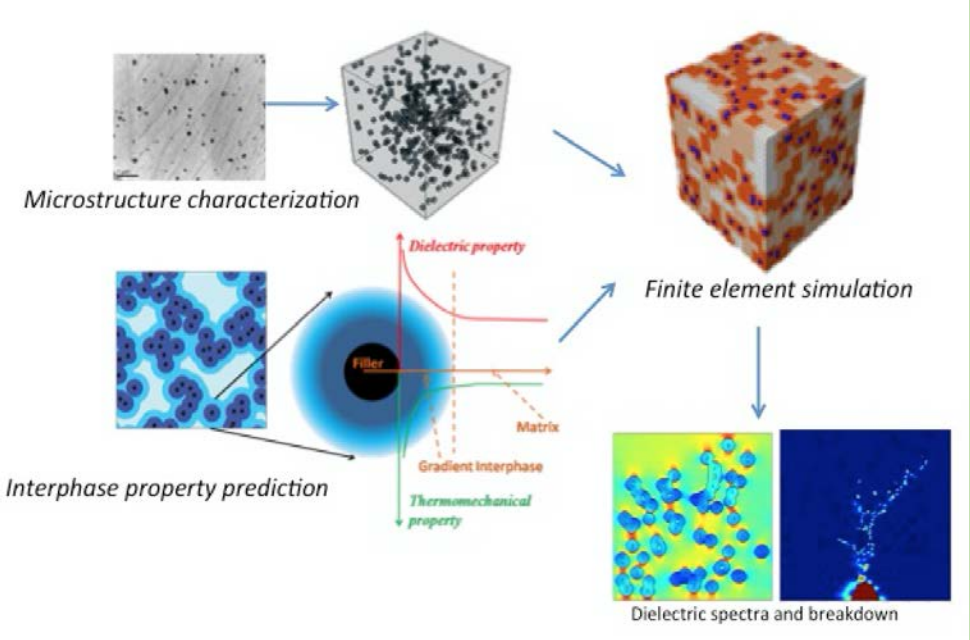
Material Property Simulation

Integrated Monte Carlo – Finite Element analysis for Charge Transport simulation[6]

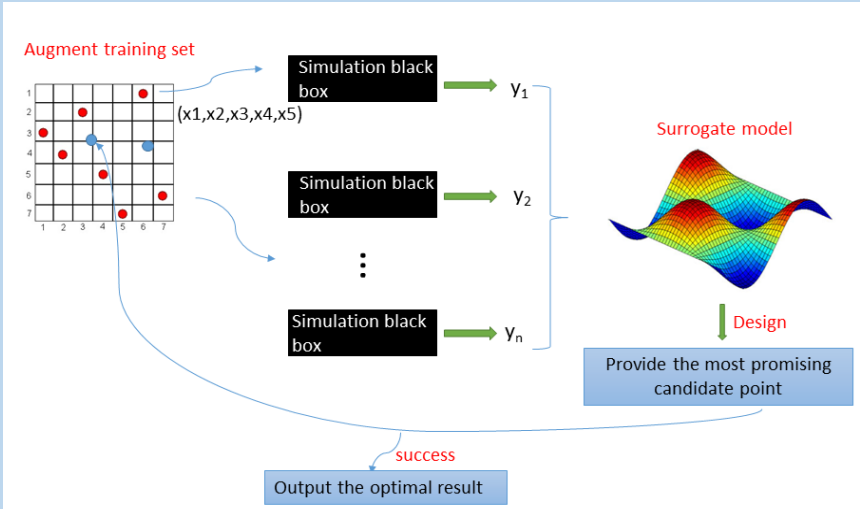


[6] Yanhui Huang, Linda. S. Schadler, arXiv,2016 (10.1063/1.4945373)

Simulating Dielectric Spectroscopy[7]



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



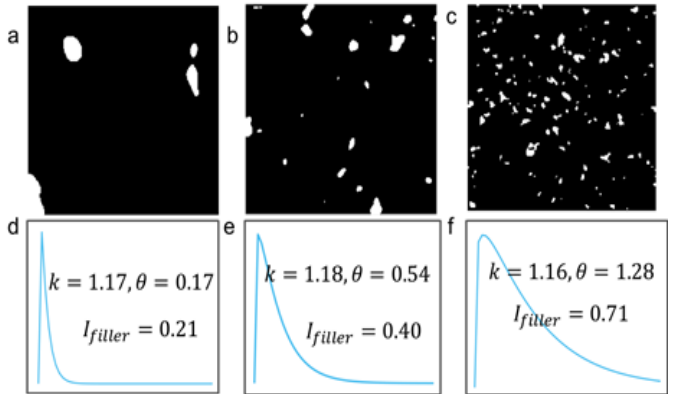
Automatic fitting of Interphase Relaxation Model[8]

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

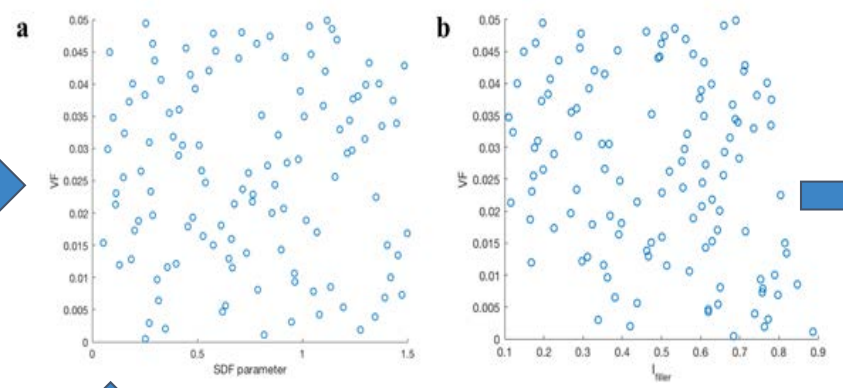
Case Study: Design of Capacitors

- 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)

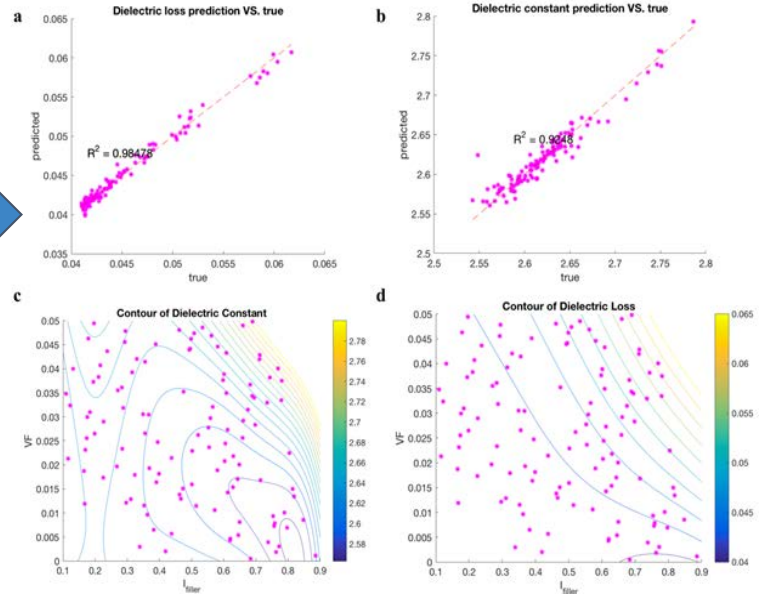
Microstructure Analysis using SDF to determine bounds of Design Variable



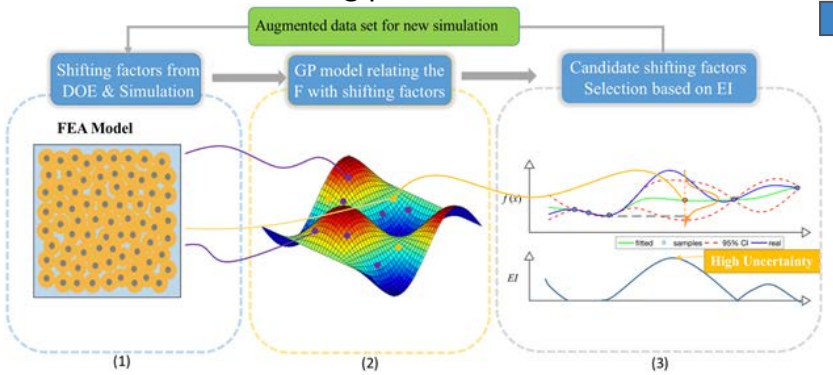
Design of Experiments using Latin Hypercube Sampling to evenly explore design space

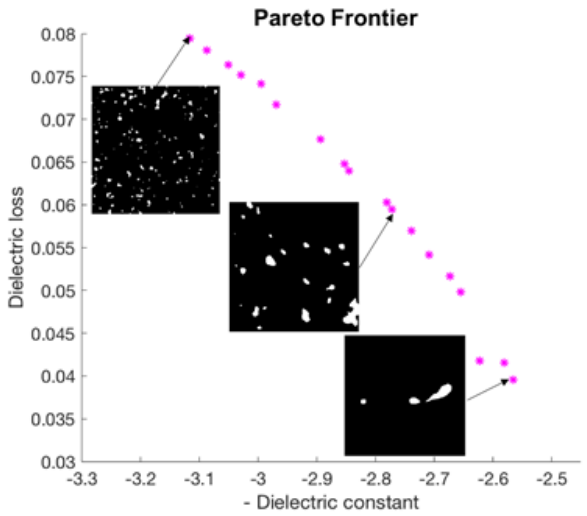


Gaussian Process Metamodel created for Dielectric constant and loss prediction to accelerate optimization



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 GI01.03 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, Metamodelling webtools to facilitate targeted design of materials

Acknowledgement

Contacts

- Prof. L Catherine Brinson (cate.brinson@duke.edu)
- Prof. Wei Chen (weichen@northwestern.edu)
- Prof. Linda Schadler (Linda.Schadler@uvm.edu)
- Prof. Deborah L McGuinness (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.