Working Group #3: Schemas of Polymer Nanocomposites

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Significance of WG's Focus

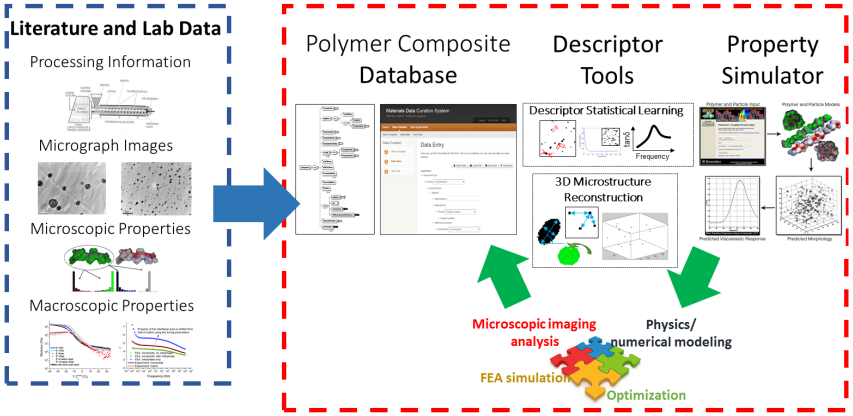
- Provide publicly available web apps of data resources and computational analysis tools for ***polymer nanocomposites*** research community

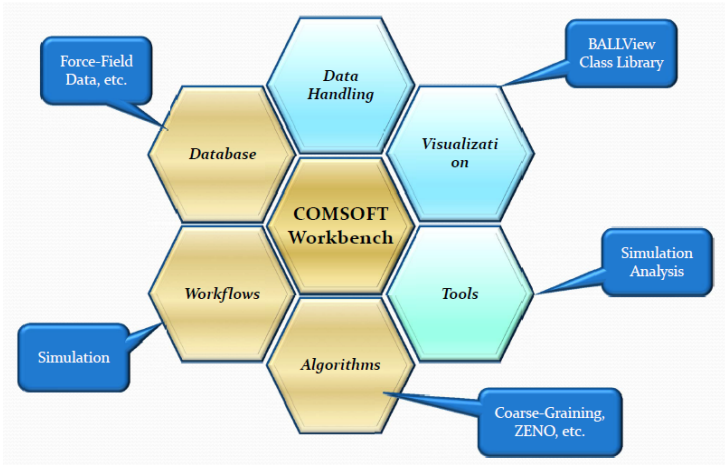
- Provide a standard of data schema for processing-structure-properties (p-s-p) experimental and computational data curation

- Case study of data mining models using available data in DB for property prediction and material design

Summary of WG's Goals

- Provide platforms and methodology for data-centered material discovery and design
  - NanoMine
    - Database
    - Analysis tools
    - Modeling
  - COMSOFT
  - Development of preliminary data analysis tools
  - Developing methods for effective TEM images processing





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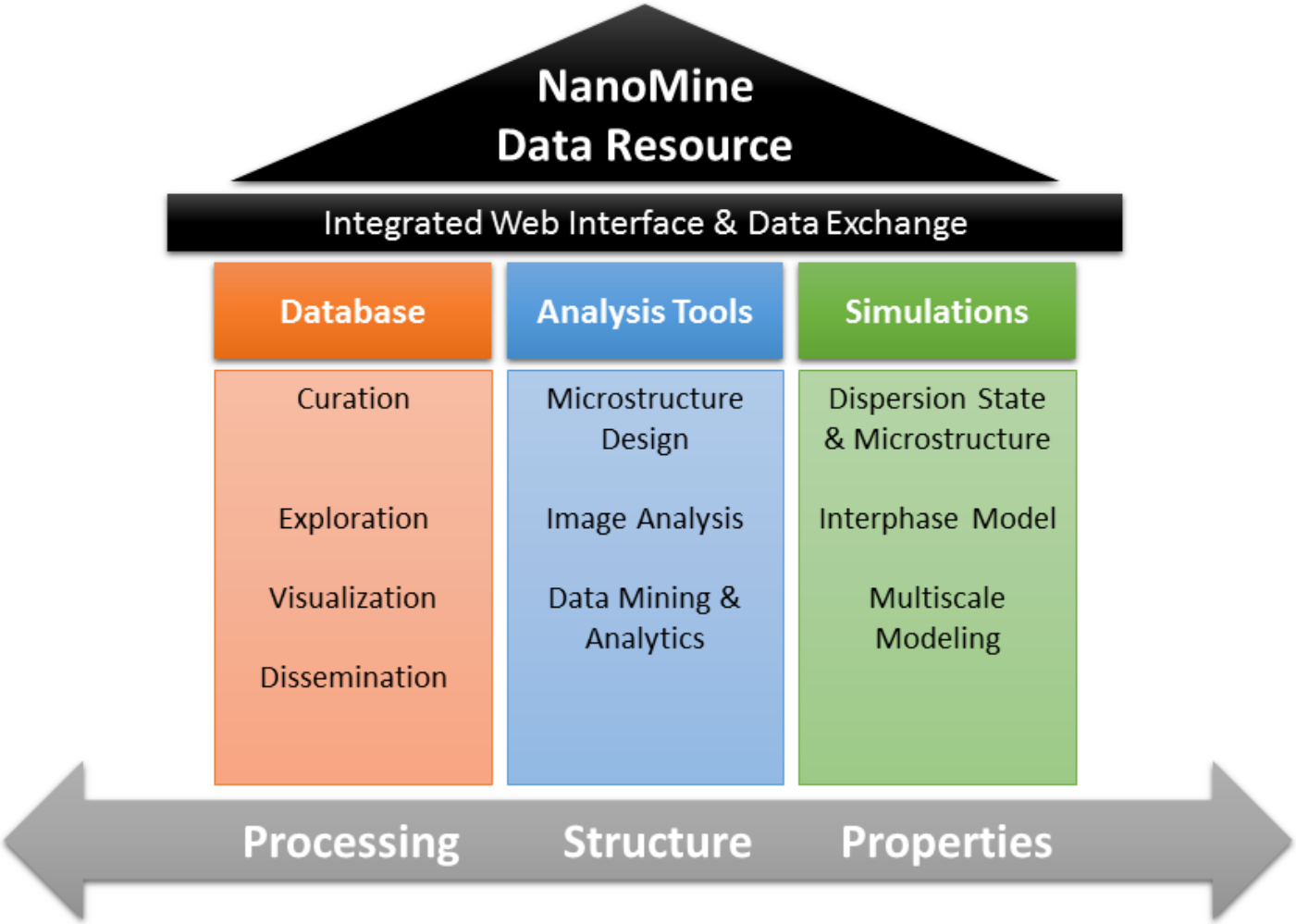
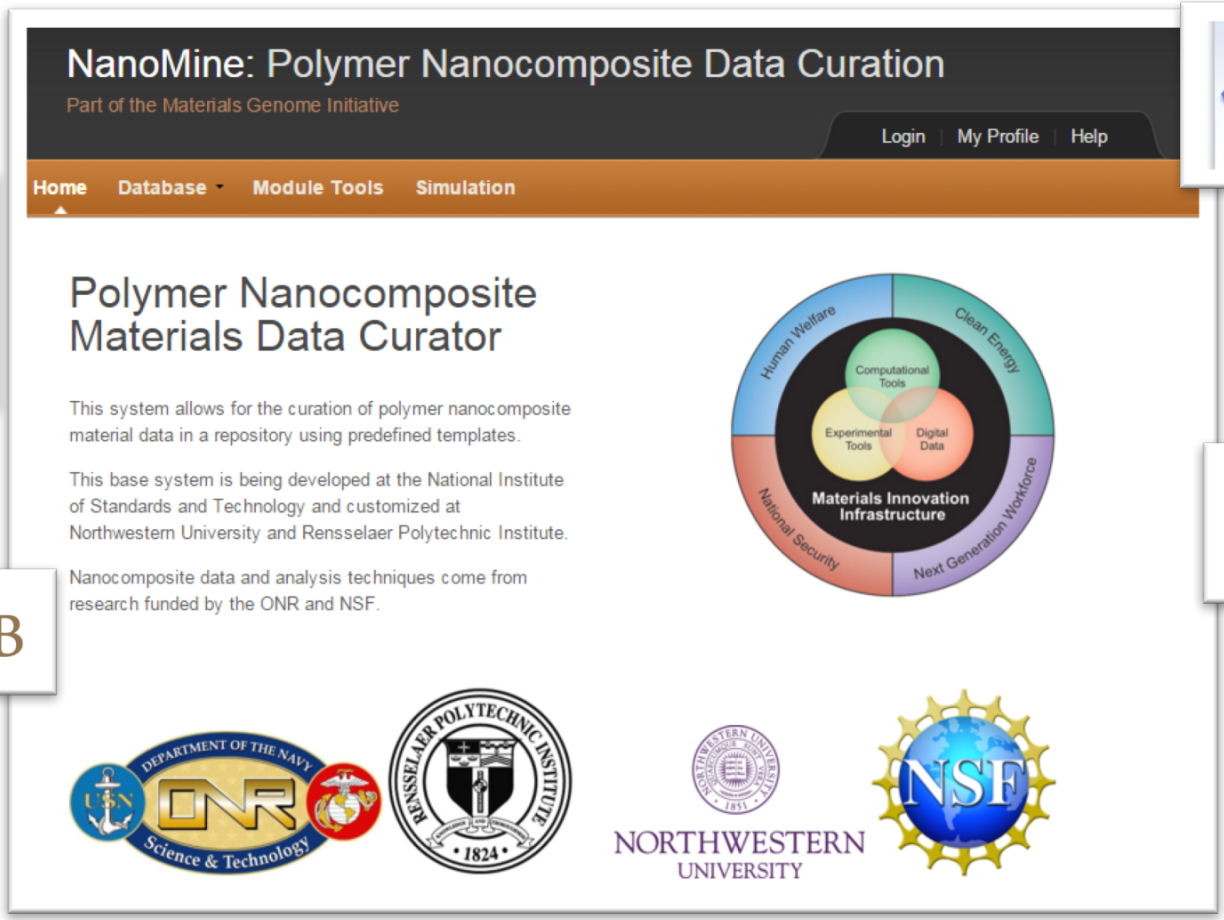
NanoMine


NanoMine
Data Resource
Integrated Web Interface & Data Exchange
Database
Analysis Tools
Simulations
Curation
Exploration
Visualization
Dissemination
Microstructure Design
Image Analysis
Data Mining & Analytics
Dispersion State & Microstructure
Interphase Model
Multiscale Modeling
Processing
Structure
Properties

Material Data Curator System



REST API

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

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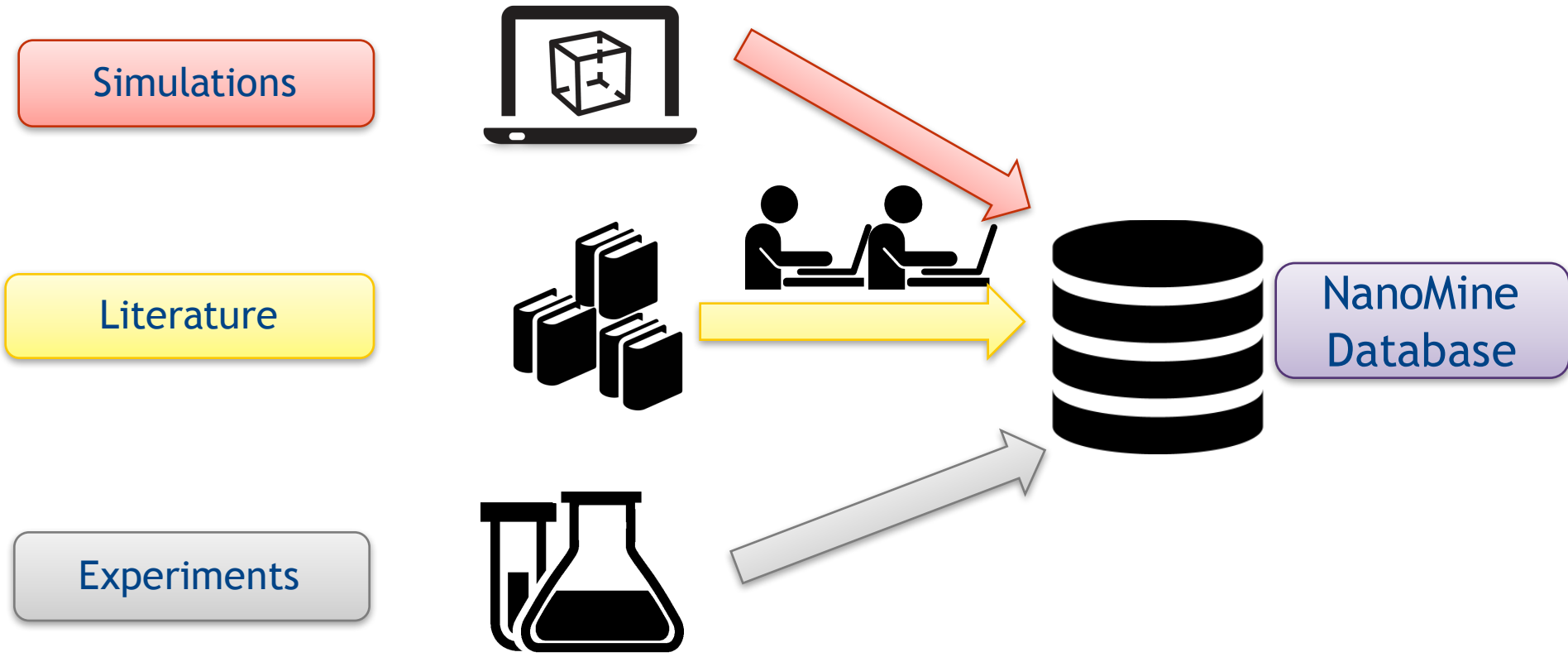
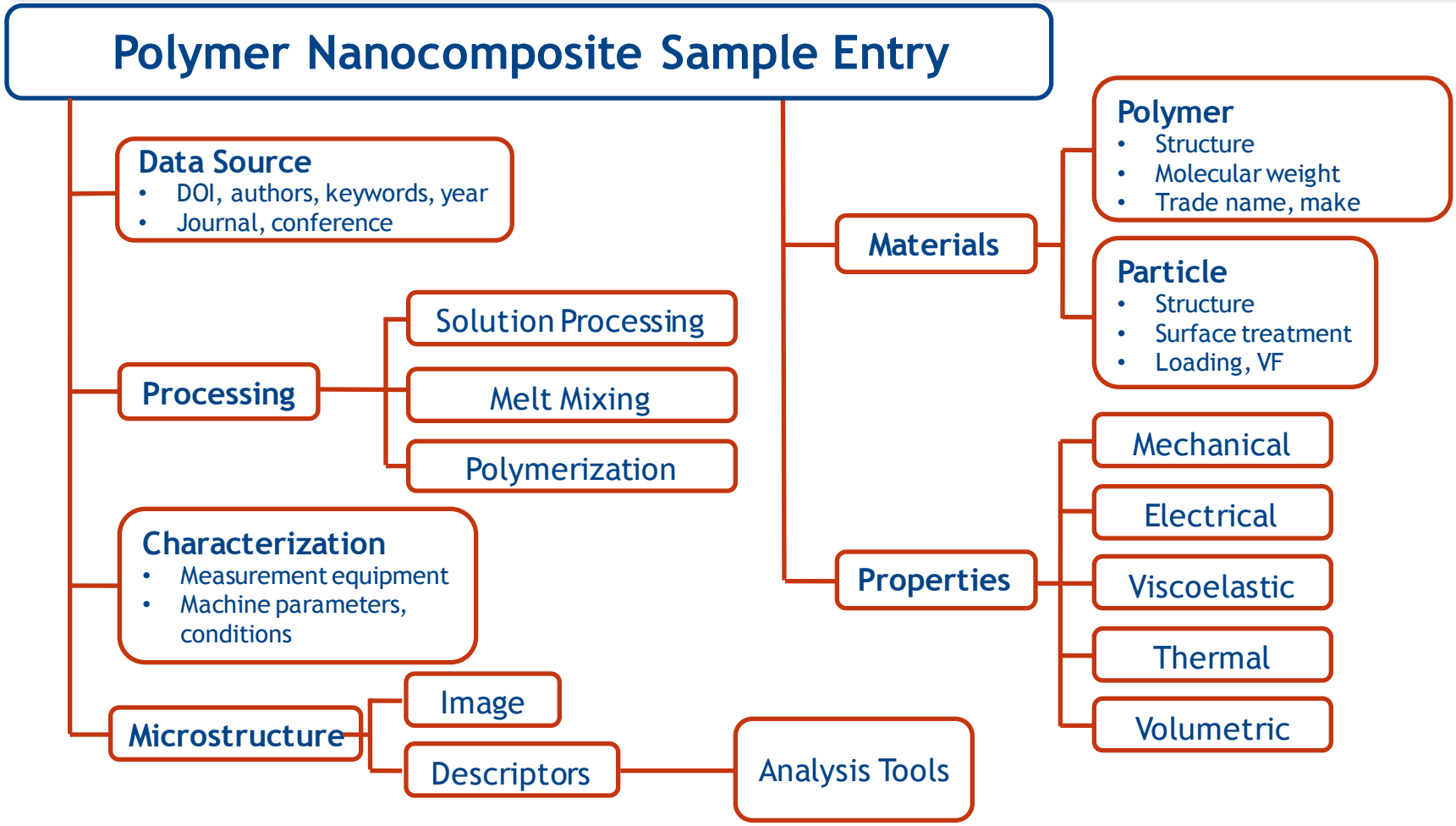
Sources of Data



XML Schema



More than 400 total attributes in current schema!

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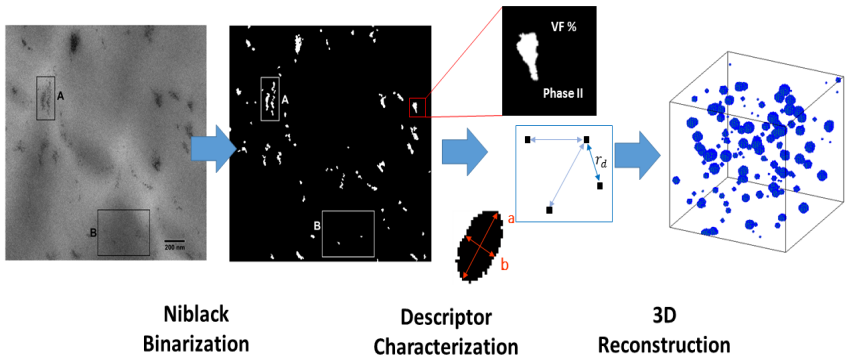
Current capabilities

- Dataset
  - 300 literature and experimental data points
  - Inorganic fillers. Viscoelastic & dielectric properties
- Tools
  - Image pre-processing
  - Microstructure characterization and reconstruction



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Technical Requirements/Needs

- Curation of literature data
- Data cleaning & formatting
- Easy user data input and contribution
- Validation of user input
- Search and statistical learning-based tools specific for material design

Collaborations/Synergies

- Other Working Groups
  - *MDCS*
    - *Web and data infrastructure*
  - *Experimental data*
    - *Data resource*
  - *NLP and DB's*
    - *Ontology & dictionary development*
  - *DFT & CALPHAD*
    - *Data analytics & material design*

Collaborations/Synergies

- NIST:
  - *Fred Phelan (WebFF, COMSOFT)*
  - *C. Campbell (MML), A. Dima (ITL)*
- *ChiMaD:*
  - *Alok Choudhary (NLP, automatic literature selection)*
  - Juan de Pablo (Polymer design database)
- *RPI:*
  - *Linda Schadler (material synthesis)*
  - *Curt Breneman (DFT, chemoinformatics)*