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NSDL
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Facilitating Wiki/Repository Communication with Metadata

International Conference on
Dublin Core and Metadata Applications
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Outline

- Background Information
  - NSDL & MatDL Pathway
- Rational
  - User Centric
  - Service Centric
- Technical Details
- Concluding Remarks

National Science, Technology, Engineering & Mathematics Education Digital Library

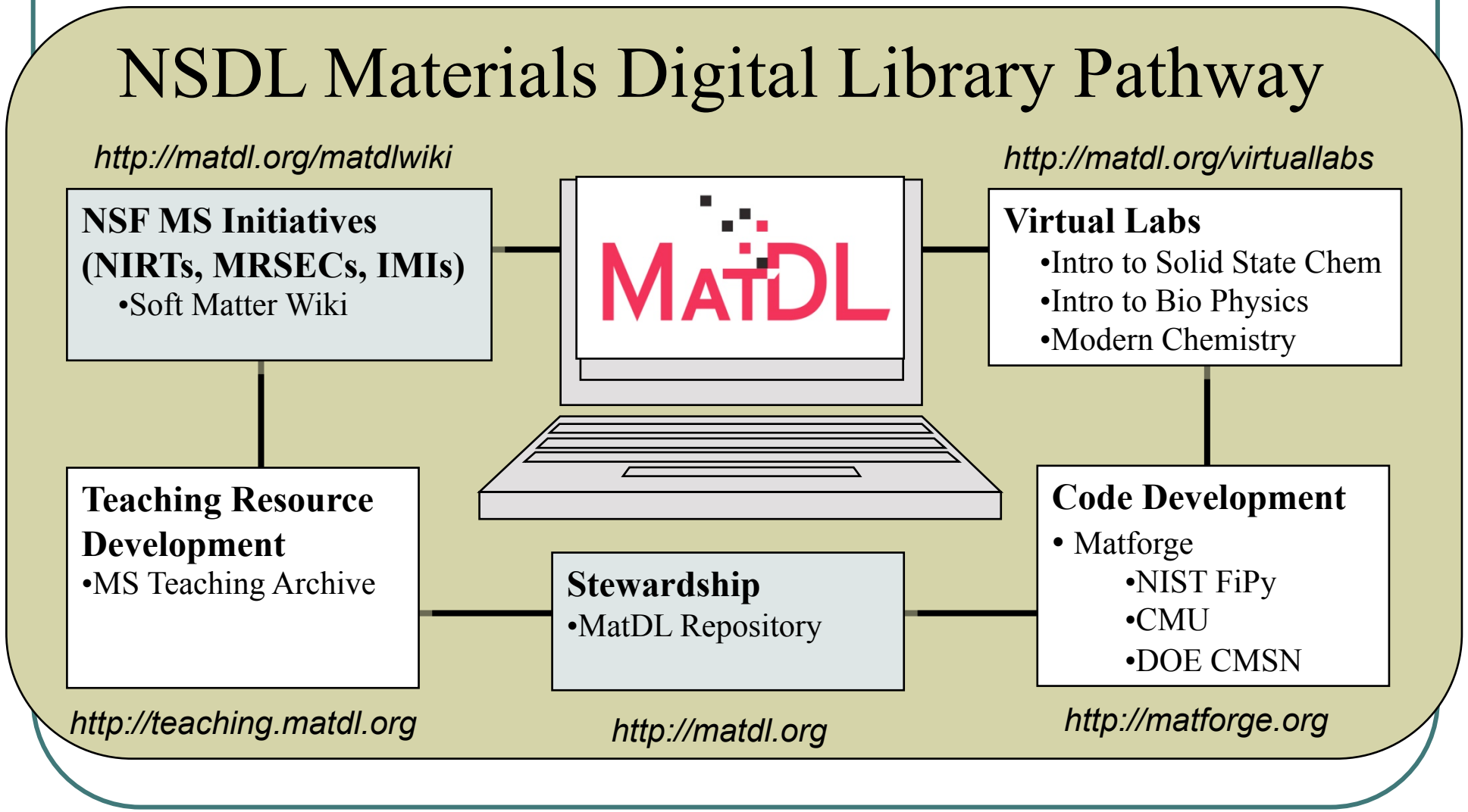
The National Science Foundation's online library of resources for education and research . . .

…established to catalyze and support continual improvements in STEM education at all levels (K-12, Higher Education, and Lifelong Learning).

Materials Digital Library Pathway

- Domain - Materials Science
  - Study of materials structure & processing-property relations to improve products
- Audience – MS research & education community
  - Undergraduate and above
- Goals
  - Implement an information infrastructure as part of NSDL
  - Disseminate information generated by government-funded efforts in materials
  - Provide content and services to support the integration of research and education in materials

NSDL Materials Digital Library Pathway

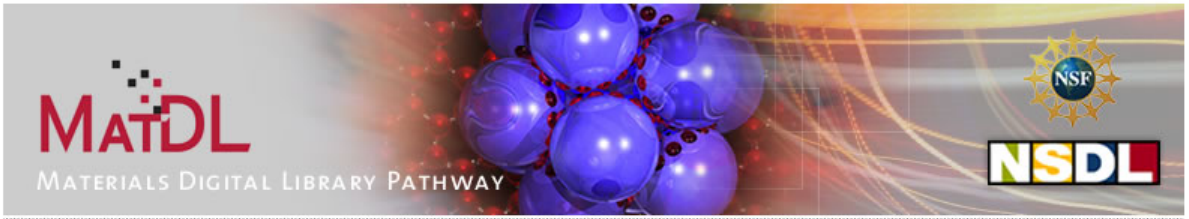


Wiki/Repository Communication

- Enable 2-way resource integration between Services: Soft Matter Wiki and MatDL Repository
  - Developed Wiki2Fedora
  - Developing Search Results plug-in

MatDL Repository

- Repository for stewardship of signigicant content
  - Fedora/Fez Installation
  - Private/public collection space
  - Externally funded resources
- Multiple purposes
  - Disseminate research & education resources
  - Support reuse & repurposing of gov't funded resources



View Conference Proceedings: ***Integrating Informatics with First Principle Calculations: Building a Materials Genome Project***

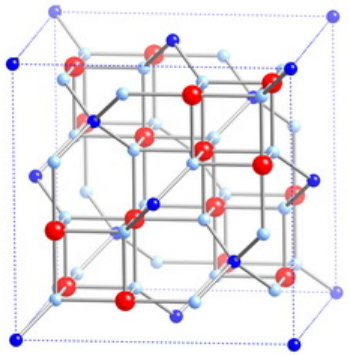
Citation: Rajan, Krishna (2007) Integrating Informatics with First Principle Calculations: Building a Materials Genome Project. In *The Third International Workshop on DFT Applied to Metals and Alloys, 2007-05-02-2007-05-04*, , Oran, Algeria:.

Collection: Combinatorial Sciences & Materials Informatics

Attached Files

Name	Description	MIMEType	Size	Downloads
A_list_of_references_for_spinel_nitrides.htm	The uploaded file is a list of references used to create a dataset of "spinel nitrides."	text/html	50.49KB	0
Description_of_spinel_variables.pdf	The uploaded file is a description of variables of "spinel nitrides" in the spinel data (excel file).	application/pdf	148.99KB	0
Oran-MatDL_slides.ppt	The uploaded file contains a powerpoint slides presented at the said conference.	application/msword	3.62MB	0
SiTi2N4.jpg	The uploaded file is a image of crystal structure of SiTi2N4, one of the "spinel nitrides."	image/jpeg	174.80KB	0
SiTi2N4.mov	The uploaded file is a movie file of crystal structure of SiTi2N4, one of the "spinel nitrides."	FFF6 0xFFF0 audio/X-HX-AAC-ADTS	174.80KB	0

Image Preview (click the image for a larger/higher quality version)



Soft Matter Wiki

- Website for use by the Soft Matter Community
  - MediaWiki Installation
  - Low-barrier collaborative authoring
  - Expert community-driven
- Multiple purposes
  - Reference resource: research lab assistants
  - Education resource: undergrad/graduate students

Soft Matter Wiki-Overview of Contents

Contents [show]

Soft Matter Wiki

[edit]

Soft materials are materials such as polymers, biomolecules, liquid crystals, surfactants, and proteins that are typically organic and can be melted and processed at moderate temperatures as compared with inorganic materials like metals and ceramics. Typically, soft materials have weak interactions among molecular or supramolecular components and are often either amorphous or can self-assemble from the liquid state. There are often many levels of complexity with heirarchical, supramolecular structures that can be cooperative and far from equilibrium. We are most often concerned with the structural arrangments, viscoelastic rheology, and/or mechanical behavior of these materials. Within these pages, you will find information pertinent to soft matter and nanomaterials, with a specific focus on computational methods and modeling.

[edit]

Course Materials

- Computational Nanoscience of Soft Matter, ChE/MSE 557 University of Michigan (Authentication Required).

[edit]

Overview of Contents

Interactions:

[edit]

Non-bonded Interactions:

[edit]

- The Lennard-Jones Potential
- Weeks-Chandler-Andersen Potential
- Hard Sphere Potential
- Dzugutov Potential
- Yukawa Potential
- van der Waals interaction
- Electrostatic interaction

Bonded Interactions:

[edit]

- Harmonic Spring
- FENE Spring
- Bond Stretching
- Angle Bending
- Bond Rotation

Simulation:

[edit]

Simulation Methods:

[edit]

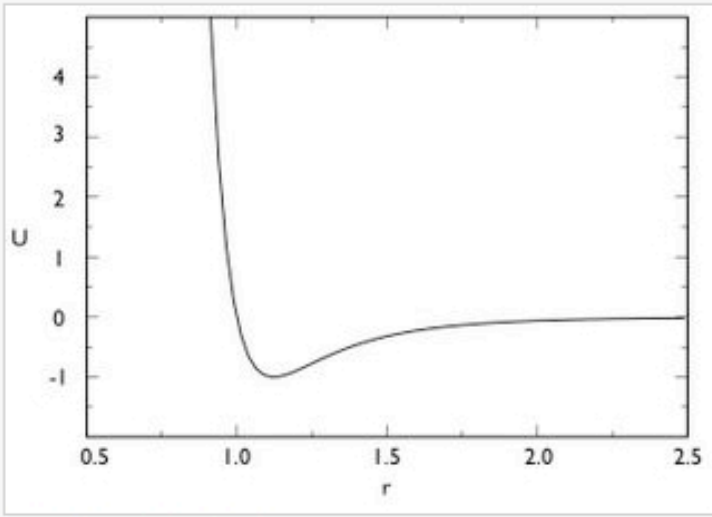
- Basic Dynamical Simulation Methodology
- Molecular Dynamics Simulation (MD)
- Brownian Dynamics Simulation (BD)

The Lennard-Jones Potential

The Lennard-Jones potential (LJ) is used to model the excluded volume interactions and van der Waals attraction of neutral atoms. The commonly used 6-12 form of the potential is as follows:

$$U_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

Where ε is the well depth, σ is the characteristic diameter (typically the diameter of the smallest particle), and *r* is the radial separation of the two atoms.



The Lennard-Jones Potential.

Contents [show]

van der Waals Attraction [edit]

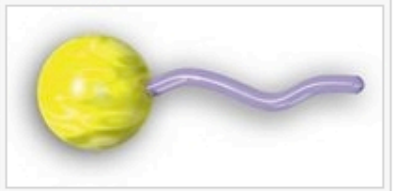
In theory, the van der Waals interaction for atoms with similar ionization frequencies and where the dispersion (London) interactions are dominant is proportional to $-\left(\frac{\alpha_{01}\alpha_{02}}{r^6}\right)$ where α01 and α02 are the polarizabilities of atom 1 and atom 2 respectively. Again, this assumes that dispersion (London) forces are dominant and that there are no permanent dipoles (Keesom forces) or induced dipoles (Debye forces). In the LJ construction, the term $\left(\frac{1}{r}\right)^6$ is used to describe this attractive van der Waals interaction.

Excluded Volume Interaction [edit]

As the seperation distance between atoms decreases, the electron clouds will eventually overlap, resulting in a very strong repulsion that rapidly increases as interatomic spacing is further decreased. In the LJ construction, the term $\left(\frac{1}{r}\right)^{12}$ describes this repulsive interaction. The 12th power is used for two main reasons: it is very steep, rapidly becoming dominant as *r* is small and it is also a multiple of the 6th power allowing for efficient computation.

Tethered Building Block

Tethered building blocks constitute a class of "shape-amphiphiles" where microphase separation occurs due to the immiscibility between the tether and building block, similar to Block copolymers and Surfactants. Building blocks can vary greatly, from metallic nanoparticles to molecular nanomaterials such as POSS or Porphyrin. Temperature, solvent quality, concentration, tether placement, number of tethers, building block geometry and composition, are only a few of the many parameters that can have a large impact on the resulting structures and phase behavior.



Cartoon of a tethered nanosphere

Experiment [edit]

Examples [edit]

- Tethered Spheres
  - *Bucky Balls*
    - Song T, Dai S, Tam KC, Lee SY, Goh SH, *Aggregation behavior of C-60-end-capped poly(ethylene oxide)s*, LANGMUIR 19 : 4798 2003
    - Song T, Dai S, Tam KC, Lee SY, Goh SH, *Aggregation behavior of two-arm fullerene-containing poly(ethylene oxide)*, POLYMER 44 : 2529 2003
  - *Quantum Dots*
    - Westenhoff S, Kotov NA, *Quantum dot on a rope*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 124 : 2448 2002
  - *Gold nanospheres*
    - Parak WJ, Pellegrino T, Micheel CM, Gerion D, Williams SC, Alivisatos AP, *Conformation of oligonucleotides attached to gold nanocrystals probed by gel electrophoresis*, NANO LETTERS 3 : 33 2003
    - Li Z, Jin RC, Mirkin CA, Letsinger RL, *Multiple thiol-anchor capped DNA-gold nanoparticle conjugates*, NUCLEIC ACIDS RESEARCH 30 : 1558 2002
    - Lu XM, Hanrath T, Johnston KP, Korgel BA, *Growth of single crystal nanowires in supercritical silicon solution from tethered gold particles on a silicon substrate*, NANO LETTERS 3 : 93 2003

Simulation [edit]

Examples [edit]

- *Tethered Spheres*
  - Z-L Zhang, M.A. Horsch, M.H. Lamm, S.C. Glotzer. *Tethered nano building blocks: Towards a conceptual framework for nanoparticle self-assembly*, Nano Letters, 3 (10): 1341-1346, (2003)
  - C.R. Iacovella, M.A. Horsch, Z-L Zhang, S.C. Glotzer. *Phase diagrams of self-assembled mono-tethered nanospheres from molecular simulation and comparison to surfactants* Langmuir, 21 (21), 9488-9494, (2005)
  - C.R. Iacovella, A.S. Keys, M.A. Horsch, S.C. Glotzer *Icosahedral packing of polymer-tethered nanospheres and stabilization of the gyroid phase* Submitted, (2006)
    - Record on MATDL Repository

Rationale: User Centric

User:

- Contributes to service providing most benefit
  - Supports user's research & teaching
- Incorporates service fitting easily into workflow
  - Easy to do and part of user's normal work
- Doesn't duplicate efforts
  - Maximizes user's time & contributions

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Rationale: Service Centric

Services:

- Accommodate user as much as possible
  - Encourages growth
- Support complex digital objects
  - Useful for research & teaching
- Describe individual objects
  - more granular, more routes of discovery
- Establish connections between services
  - Maximizes gains for user & services

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Wiki → Repository: Wiki2Fedora

- Wiki (MediaWiki)
- Repository (Fedora/Fez)
- Wiki2Fedora application
  - Runs at scheduled intervals
  - Identifies new/changed Wiki file uploads
  - Extracts available metadata from Wiki
  - Converts to DC metadata
  - Ingests datastream into Fedora

Wiki → Repository: Wiki2Fedora

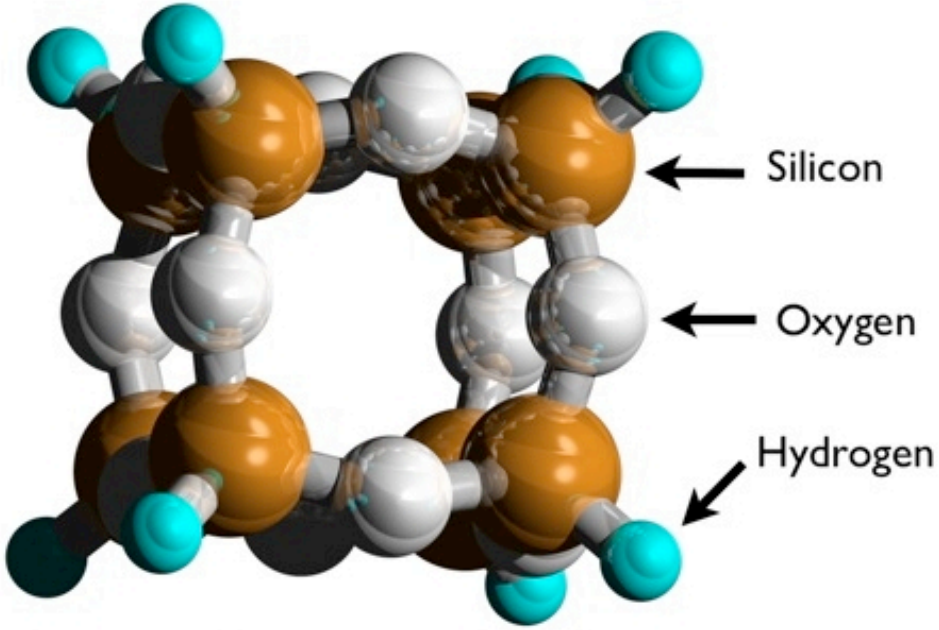
- Post-processing
  - FEZ Administration function
    - Index new objects into Fez
    - Send items to review area for manual editing /augmenting

Wiki → Repository: Wiki2Fedora

MediaWiki	DC element
filename	DC:title
comments	DC:description
file upload date	DC:date
user name→full name	DC:creator
general rights statement	DC:rights
affiliation	DC:publisher
links	links

Image:POSS.jpg

Image | File history | Links



No higher resolution available.
POSS.jpg (451 × 299 pixel, file size: 43 KB, MIME type: image/jpeg)
Schematic of a POSS cage

File history

Click on a date/time to view the file as it appeared at that time.

Date/Time	User	Dimensions	File size	Comment
(delete all) (current) 16:21, 23 September 2006	Cri (Talk | contribs | block)	451×299	43 KB	Schematic of a POSS cage

- Upload a new version of this file
- Edit this file using an external application

See the setup instructions for more information.

Links

The following pages link to this file:

- softmatter:POSS

Wiki Image & Metadata Display

POSS - Fez | NSDL Materials Digital Library Soft Mat...

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Materials Digital Library Pathway

NSF NSDL

Guest - March 27, 2008 | Administration | Browse Communities | Register | Logout | Help

View Image: *POSS*

Workflows:

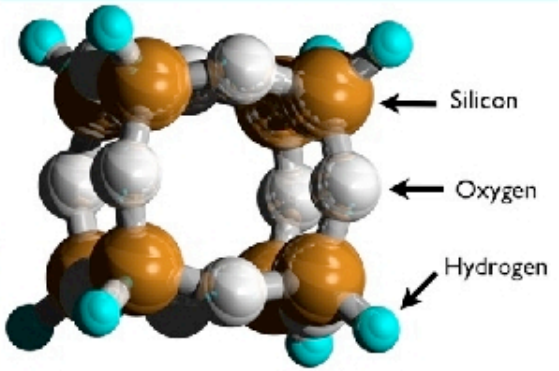
Citation: Chris Iacovella (2006). *POSS*. Glotzer group. Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics, University of Michigan.

Collection: Lab for Computational Nanoscience and Soft Matter Simulation (2006 - Present)

Attached Files

Name	Description	MIMEType	Size	Downloads
wiki2fez2462.jpg	POSS.jpg	image/jpeg	43.36KB	0

Image Preview (click the image for a larger/higher quality version)



NOTE: This record is not published.

Title	POSS
Creator(s)	Chris Iacovella
Abstract/Summary	Schematic of a POSS cage
Publisher	Glotzer group. Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics, University of Michigan
Date	2006-09-23
Source	Soft Matter Wiki
Rights	http://creativecommons.org/licenses/by-nc-sa/3.0/

Related Links

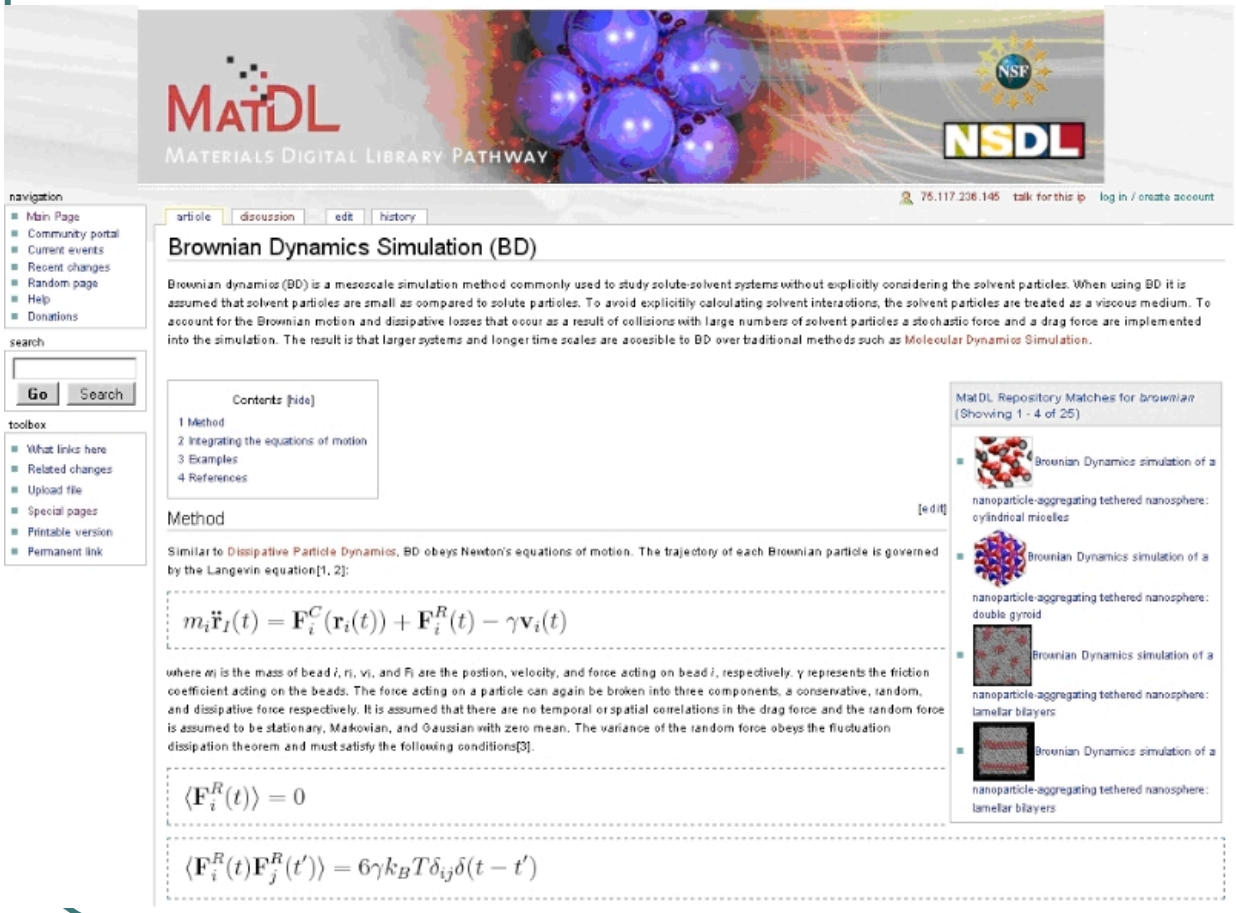
Link	Description
http://matdl.org/matdlwiki/index.php?title=softmatter:POSS	referring wiki page

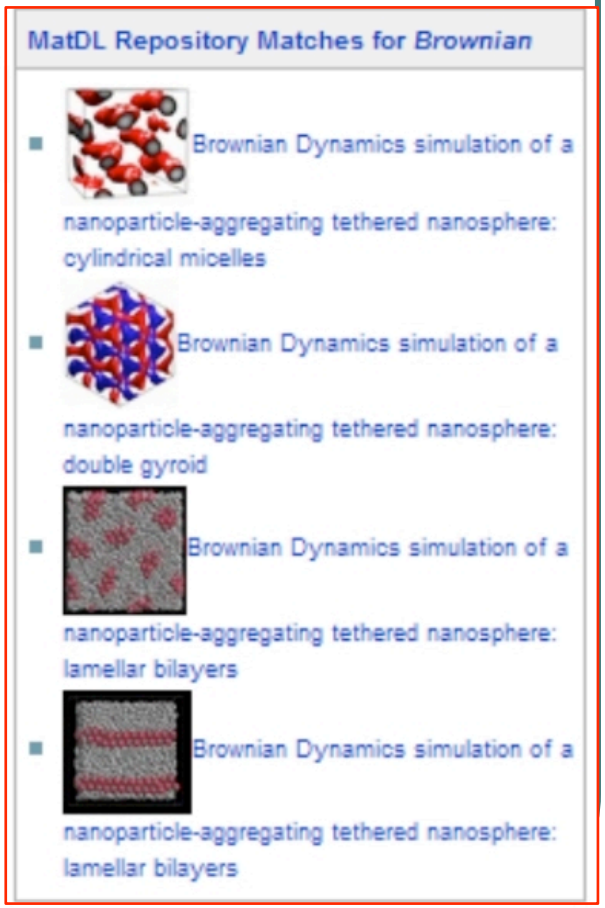
Repository Image & Metadata Display

Repository → Wiki: Search Results Plugin

- Displays Repository search results in Wiki
- MediaWiki markup extended
- Parameters <fez>
  - Query terms
  - Display
- Uses existing Fez search function

Repository → Wiki: Search Results Plugin





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Concluding Remarks

- Provide services to support collaboration & to hold authoritative scientific content
- Better integrate services
  - Avoid duplication of effort
  - Increase discovery
  - Capitalize on strengths of individual services
- Extend wiki/repository communication to other wiki software

Thank you & Questions?

lbartolo@kent.edu clowe@kent.edu

MatDL Repository	http://matdl.org
Soft Matter Wiki	http://matdl.org/matdlwiki

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