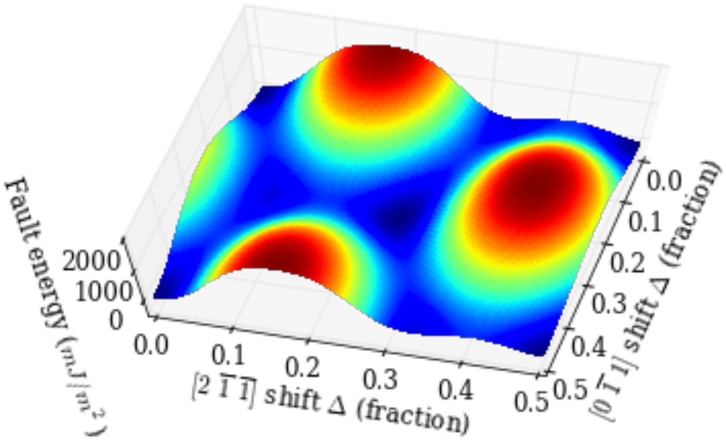
Atomistic Simulations for Industrial Needs

August 5-7, 2020

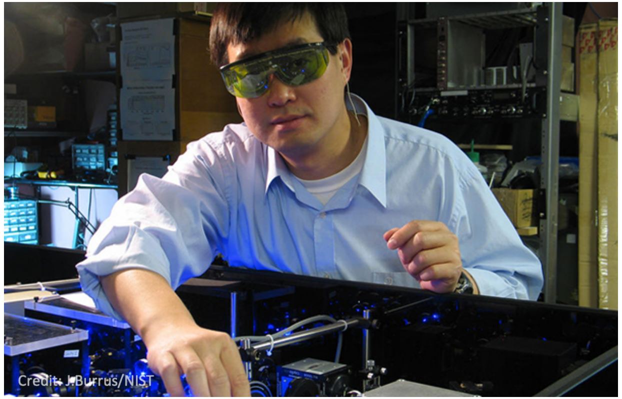


National Institute of Standards and Technology
U.S. Department of Commerce

MATERIAL MEASUREMENT LABORATORY

NIST MISSION

To promote U.S. innovation and industrial competitiveness by advancing **measurement science, standards, and technology** in ways that enhance economic security and improve our quality of life



MEASUREMENTS ESSENTIAL TO COMMERCE, TRADE, AND INNOVATION

Federal role established in the U.S. Constitution

INNOVATION

The patent system … added the fuel of interest to the fire of genius in the discovery and production of new and useful things.

Abraham Lincoln – April 6, 1858

U.S. Patent No. 6469

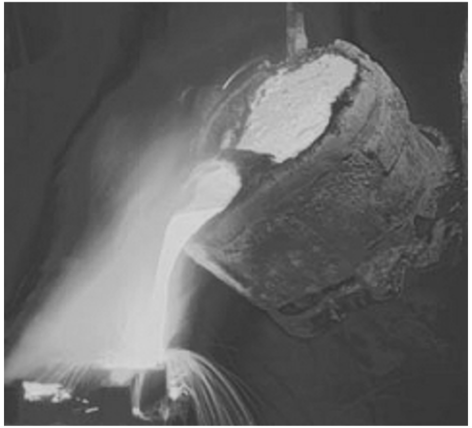
…Giving effectual encouragement as well to the introduction of **new and useful inventions** from abroad as to the exertions of skill and genius in producing them at home, and of facilitating the intercourse between the distant parts of our country…

George Washington, State of the Union Address, January 8, 1790

EARLY DRIVERS FOR STANDARDS AND MEASUREMENTS

1904

Out-of-town fire companies arriving at a Baltimore fire cannot couple their hoses to the hydrants. 1526 buildings razed.



1905

Standard samples program begins with standardized irons.

1912

41,578 train derailments **in the previous decade lead to NBS measurement and test program.**

NIST AT A GLANCE

Industry's National Laboratory

3,400+
FEDERAL EMPLOYEES

5
NOBEL PRIZES

2 CAMPUSES
GAITHERSBURG, MD [HQ]
BOULDER, CO

3,500+
ASSOCIATES

10
COLLABORATIVE
INSTITUTES

400+
BUSINESSES USING NIST FACILITIES

14
NATL OFFICE FOR MANUFACTURING INSTITUTES

ManufacturingUSA

51
MANUFACTURING EXTENSION PARTNERSHIP CENTERS

U.S. BALDRIGE PERFORMANCE EXCELLENCE PROGRAM

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

REDEFINING THE WORLD’S MEASUREMENT SYSTEM: SI UNITS

On November 16, 2018, at Versailles, France, the world’s scientific and technical community redefined four of the seven base units for the International System of Units (SI). The affirmative vote means the kilogram (mass), kelvin (temperature), ampere (electric current) and mole (amount of substance) are now determined by fundamental constants of nature instead of by physical objects. This historic change is the largest single shift in international measurement since the Treaty of the Meter was signed in 1875. Scientists expect this change will spur technological innovation and lower the cost of many high-tech manufacturing processes.

NIST Priority Research Areas

Advanced manufacturing

Fotocrisis/shutterstock

IT and cybersecurity

Designersart/shutterstock

Bioeconomy

Quantum Science

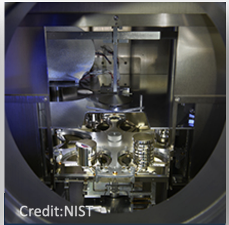
Artificial Intelligence

Internet of Things

Infrastructure Resilience

NIST LABORATORY PROGRAMS

Material Measurement Laboratory

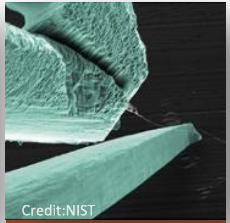


Physical Measurement Laboratory

Engineering Laboratory

Information Technology Laboratory

Communication Technology Laboratory



Center for Nanoscale Science and Technology

NIST Center for Neutron Research

Material Measurement Laboratory

Measurement science, technology, standards, models and data that support…

Materials Science and Engineering (MSED)

Materials Measurement Science (MMSD)

Biosystems and Biomaterials (BBD)

Biomolecular Measurement (BMD)

Chemical Sciences (CSD)

Applied Chemicals and Materials (ACMD)

Materials

MSED: design, development, manufacture, and use of materials by industry.

MMSD: next-generation characterization of materials ID, structure, composition and properties on all scales.

Bioscience

BBD: quantification of biological systems, materials and processes, from the nano to macro-scale.

BMD: determination of the composition, structure, quantity, and function of biomolecules, including protiens, DNA, lipids and metabolites.

Chemistry

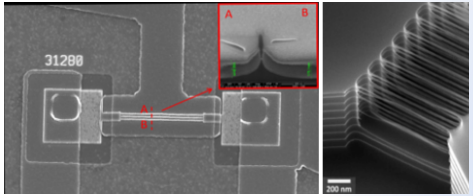
CSD: determination of chemical composition and structure of gases, organic, and inorganic species, properties and processes, reactivity and mechanisms.

ACMD: design, production, and assessment of chemical and material products, with a focus on reliability.

NIST MATERIAL MEASUREMENT LABORATORY

Measurements of composition, structure & properties of matter…
…to advance technologies that serve all of humankind

Advanced Electronics



Reliable Materials for Buildings and Vehicles

Assessment of Soil, Water and Air Quality

Accurate Measurement of Materials, Chemicals & Biological Substances

Clean Alternative Fuels

Science-based DNA and Physical Forensics

Trustworthy Medical Tests and Diagnoses

NIST Products and Services

Collaborations

- 2600 Associates and Facility Users

Measurement Research

- 2,200 publications per year
- 8,000 attendees at 69 technical conferences

Standard Reference Data

- 100 different types
- 6,000 units sold per year
- 130 million data downloads per year

Standard Reference Materials

- 1,300 products available
- 33,000 units sold per year

Calibration Tests

- 24,000 tests per year

Laboratory Accreditation

- 800 accreditations of testing and calibrations laboratories per year

Standards Committees

- 400 NIST staff serving on 1,000 national and international standards committees

CENTER OF EXCELLENCE FOR ADVANCED MATERIALS RESEARCH

Center for Hierarchical Materials Design (CHiMaD)- led by Northwestern University

Consortium Members

- Northwestern-Argonne Institute of Science and Engineering
- Computation Institute (a partnership between the University of Chicago and Argonne)

Others closely involved include

- QuesTek Innovations
- ASM International

Northwestern University
Evanston, IL

Focus: developing the next generation of computational tools, databases and experimental techniques to enable "Materials by Design"

MATERIALS SCIENCE AND ENGINEERING

Division Function:

Division Chief: Mark VanLandingham

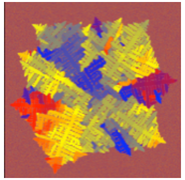
Provides the measurement science, standards, technology, and data required to support the Nation's need to design, develop, manufacture, and use materials.

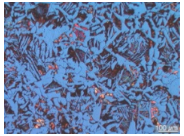
Groups:

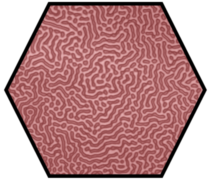
- Polymers & Complex Fluids (Kate Beers)
- Functional Polymers (Chris Soles)
- Functional Nanostructured Materials (Albert Davydov)
- Mechanical Performance (Jon Guyer)
- Thermodynamics and Kinetics (Carrie Campbell)
- Polymer Processing (Dean DeLongchamp)

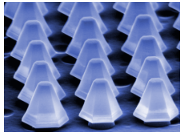
Capabilities:

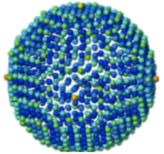
- Metallurgical materials science (e.g. alloys, solidification, processing)
- Polymer & colloidal materials science (e.g. carbon nanotubes, nSoft)
- Microstructure, nanostructure (e.g. microscopy, scattering)
- Mechanical performance (NCAL, ballistic fibers)
- Materials data and computational tools (MGI)





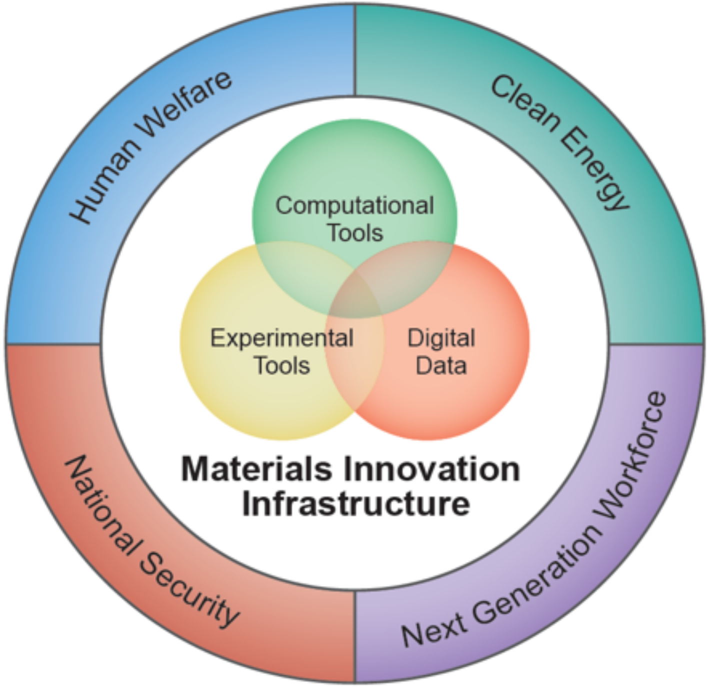






The Materials Genome Initiative

Goal: to decrease time-to-market by 50% while <$$



Develop a Materials Innovation Infrastructure

Achieve National goals in energy, security, and human welfare with advanced materials

Equip the next generation materials workforce

Materials Genome Initiative for Global Competitiveness

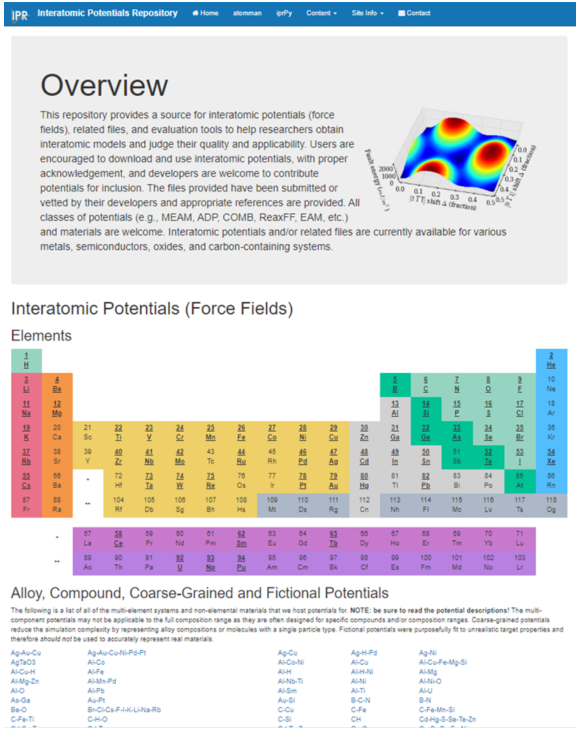
INTERATOMIC POTENTIALS

Workshop history:

- Started in 2008 by Chandler Becker to bring together industry, government and academia to address the current state of the art and identify currents needs and challenges.
- Held annually from 2008-2014 (https://www.ctcms.nist.gov/potentials/activities.html)
  - 2012: MGI focus
  - 2013: Testing and Validation focus
  - 2014: Materials for Gas Separations; Metal-Organic Frameworks
  - 2018: Potential Development and Workflow tools
-

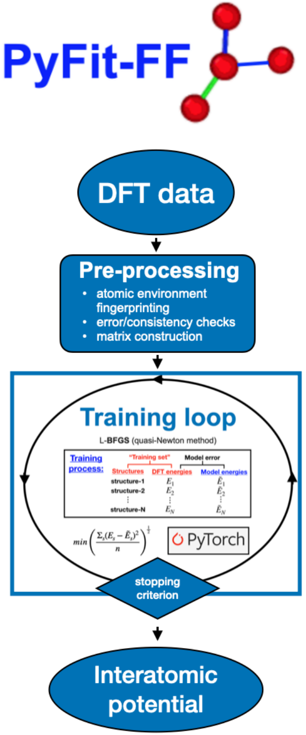
Interatomic Potential Development and Tools at NIST

- Interatomic potential repository (IPR)
- Atomman
- iprPy
- PyFit-FF
- PINN potentials
- JARVIS-FF

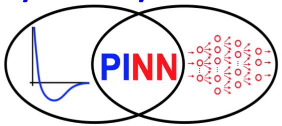


www.ctcms.nist.gov/potentials

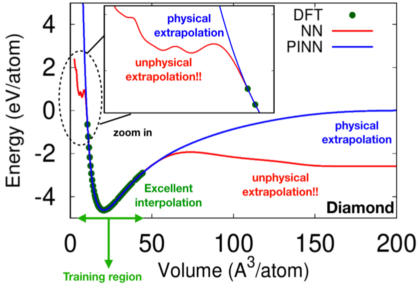
PyFit-FF



Physically informed



Neural Network potentials



LOGISTICS

Schedule

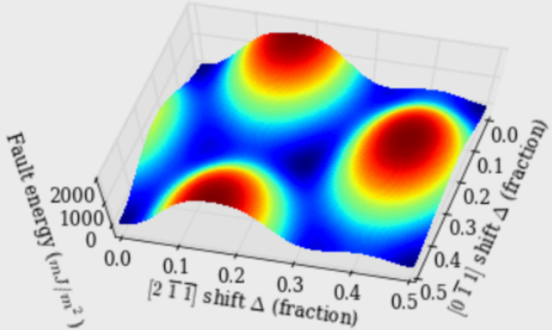
Session interactions

Lunch

Notice! This site is currently under construction and testing.

New! Please give us your feedback

Overview



This repository provides a source for interatomic potentials (force fields), related files, and evaluation tools to help researchers obtain interatomic models and judge their quality and applicability. Users are encouraged to download and use interatomic potentials, with proper acknowledgement, and developers are welcome to contribute potentials for inclusion. The files provided have been submitted or vetted by their developers and appropriate references are provided. All classes of potentials (e.g., MEAM, ADP, COMB, Reax, EAM, etc.) and materials are welcome. Interatomic potentials and/or related files are currently available for various metals, semiconductors, oxides, and carbon-containing systems.