CSSI Framework: Cyberloop for Accelerated Bionanomaterials Design

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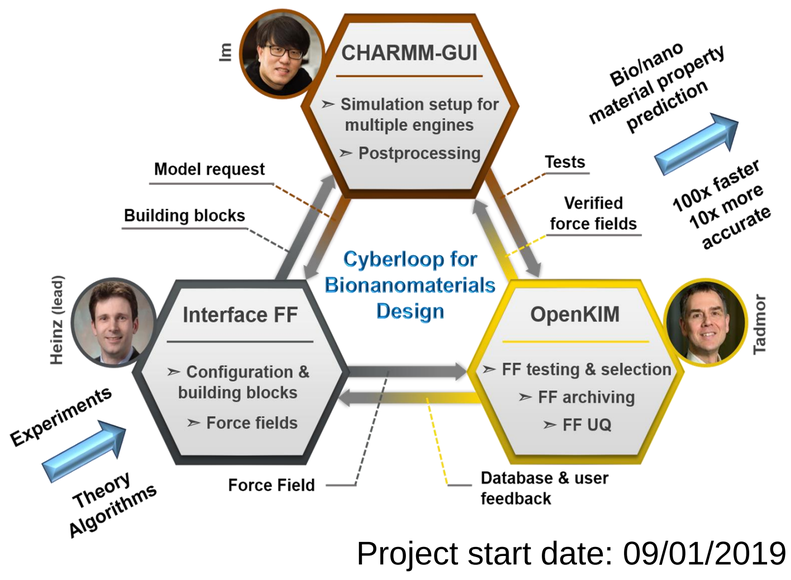
Award #: 1931587

Objective

Merge 3 major existing community programs with 10+ year usage record for open source, accurate simulations of nanomaterials and biomaterials.



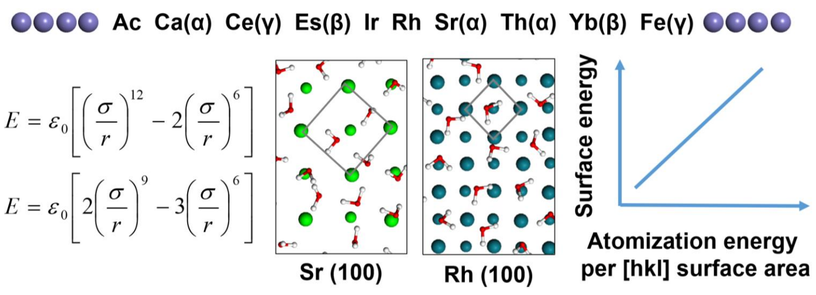
Project start date: 09/01/2019

Supported Nanomaterials from IFF

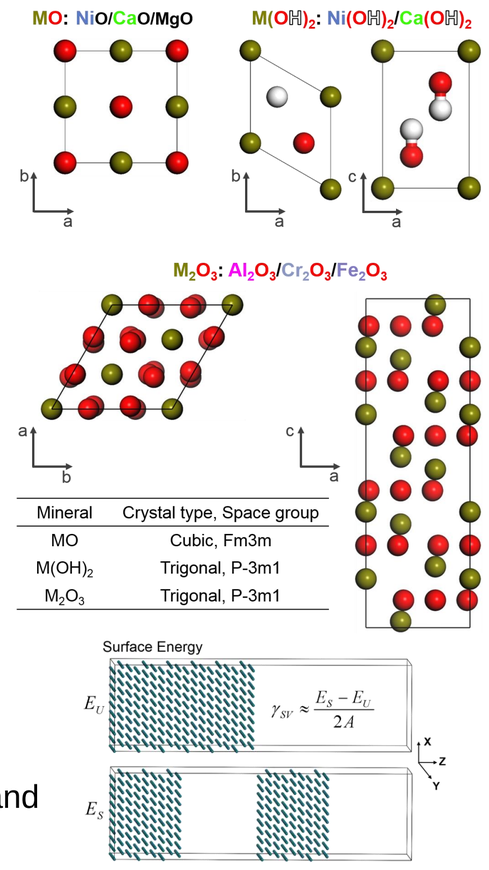
https://bionanostructures.com/interface-md/

- Fcc metals: Ag, Al, Au, Cu, Ni, Pb, Pd, Pt bulk minerals, including different cleavage planes (up to 3), a variety of shapes (i.e., sphere, cylinder, rod, polygon, and box), and Wulff construction. In particular, ligand-protected Au nanocluster/nanoparticle/surface are also provided.
- Clay Minerals: Kaolinite ($Al_2Si_2O_5(OH)_4$) and Montmorillonite $(K, Na)_n[Si_4O_8][Al_{2-n}Mg_nO_2(OH)_2]$. In the case of Montmorillonite, users can control the contents of Mg defect and ion types.
- Mica: Muscovite ($KAl_2(AlSi_3)O_{10}(OH)_2$).
- Calcium Sulfates: Gypsum ($CaSO_4 \cdot 2H_2O$), Hemihydrate ($CaSO_4 \cdot 1/2H_2O$), and Anhydrite ($CaSO_4$) with different cleavage planes and Wulff construction.
- Cement Minerals: Tricalcium Silicate (Ca_3SiO_5) and Tricalcium Aluminate ($Ca_3Al_2O_6$) with different cleavage planes and Wulff construction.
- Calcium Silicate Hydrate: Tobermorite ($Ca_4Si_6O_{15}(OH)_2 \cdot 5H_2O$).
- Silica: bulk minerals (α-quartz, α-cristobalite) as well as surfaces of different degree of ionization for specific pH values and particle sizes
- Phosphate Minerals: bulk mineral of Hydroxyapatite ($Ca_5(PO_4)_3(OH)$), different cleavage planes and Wulff construction for various pH.
- Carbonaceous Materials: Carbon Nanotube, Graphene, and Graphite.

Newly Added Metals and Oxides



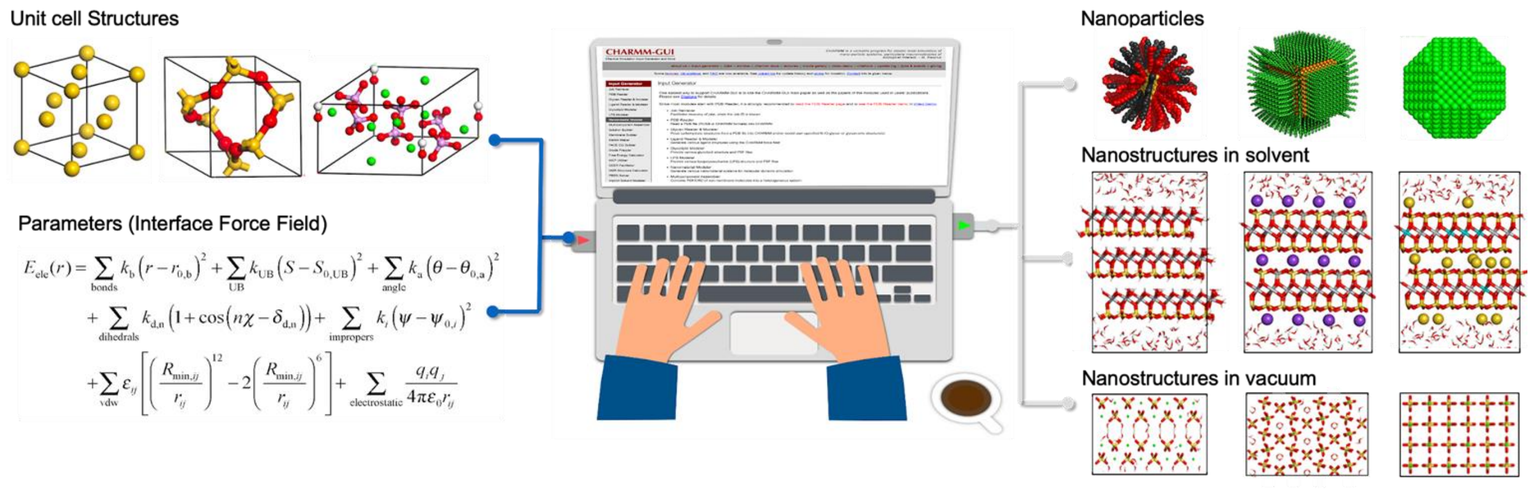
- Provide force field, structures, and IFF surface model database to CHARMM-GUI and Nanomaterial Modeler
- Assist OpenKIM with standardizing protocols for property calculations in LAMMPS: cell parameters, surface energy, hydration energy, mechanical properties at 298 K and 101 kPa
- Assisting in testing and quality improvement



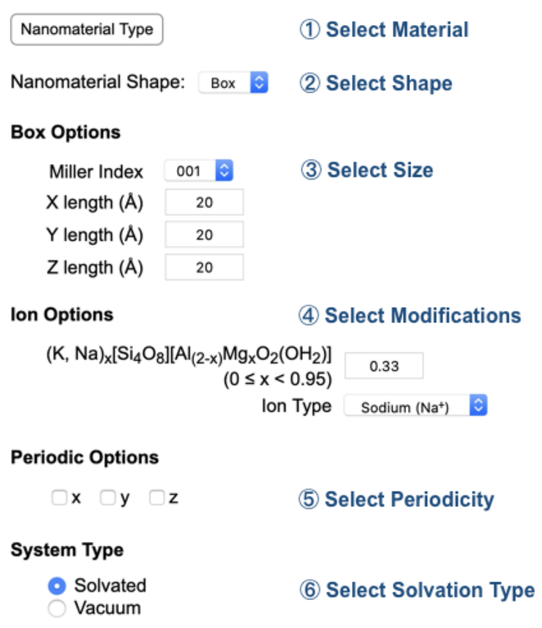
Mineral	Crystal type, Space group
MO	Cubic, Fm3m
$M(OH)_2$	Trigonal, P-3m1
M_2O_3	Trigonal, P-3m1

Working Scheme of CHARMM-GUI Nanomaterial Modeler

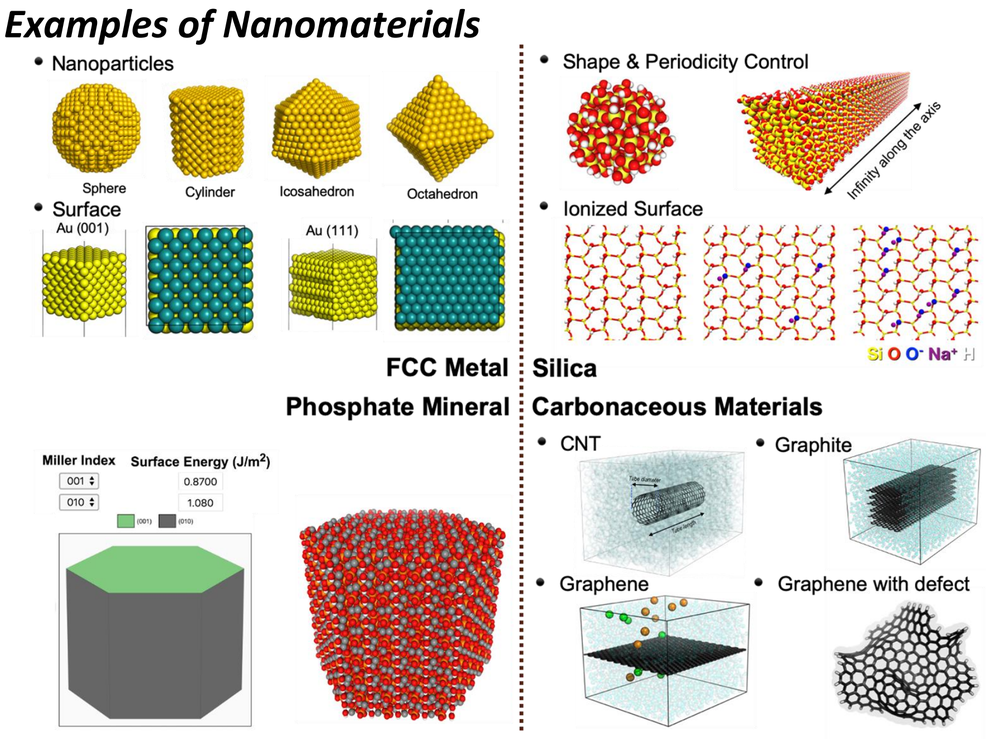
http://www.charmm-gui.org/?doc=input/nanomaterial



User Inputs



Examples of Nanomaterials



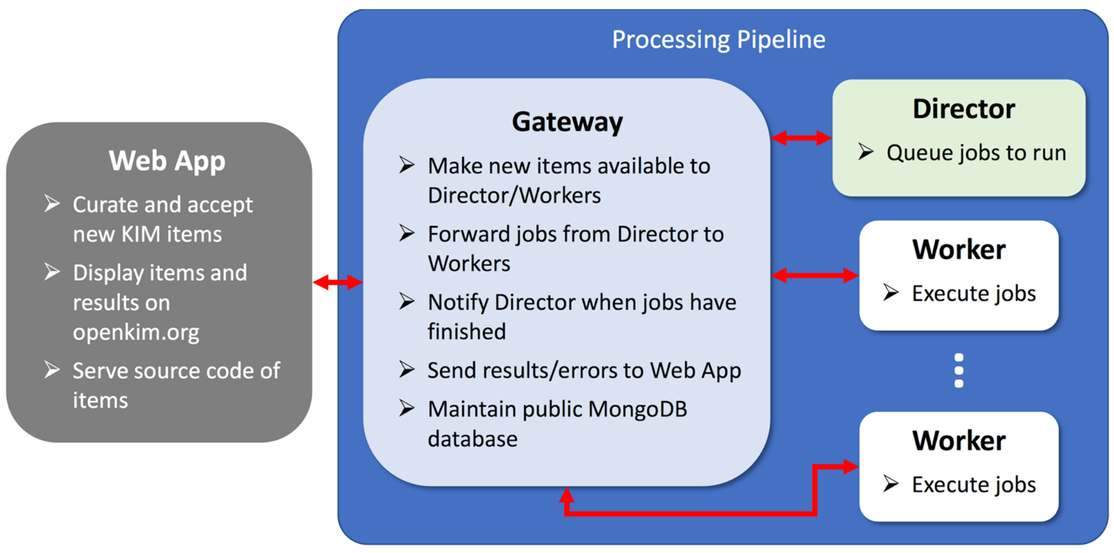
- Automatic generation of simulation-ready files in different formats: LAMMPS, NAMD, GROMACS, OpenMM
- Next step: automated integration of biomacromolecules into model building

Curating and testing of force fields on OpenKIM https://openkim.org/

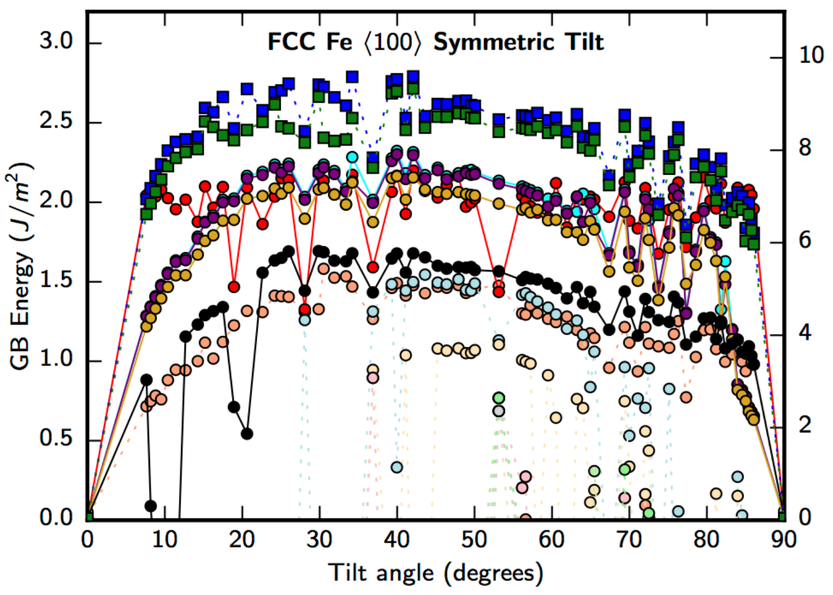
The **Open Knowledgebase of Interatomic Models project** curates force fields (FFs) with full provenance control, issues them DOIs so that they can be cited in publications, and tests them exhaustively using "KIM Tests" that compute a host of material properties and "Verification Checks" (VCs) on coding correctness. FFs archived in OpenKIM conform to the KIM Application Programming Interface (API) that allows them be used in plug-and-play fashion with a variety of major simulation codes. The overall aim of the project is to improve the reliability and reproducibility of molecular simulations of materials including bionanomaterial systems.

Overview of OpenKIM Structure: Users interact with OpenKIM through a website where they can upload/download FFs and visualize Test and VC results.

An FF uploaded to OpenKIM is run against all compatible Tests and VCs in the system using an automated **Processing Pipeline** framework, which consists of a cloud-based system of a Gateway, Director, and workers that perform the computations.



- First simulator models for bonded potentials (IFF) were built and tested, adding a new category of widely used force fields into OpenKIM
- Standardized property validation protocols (surface energies, hydration energies, mechanical) in progress



Runnels et al, in preparation (2020).

Example: Comparison of FF prediction for grain boundary (GB) excess energy in FCC Fe as a function of symmetric tilt angle about the <110> axis for FFs in OpenKIM.