

GULP

The General Utility Lattice Program, or GULP, is a classical simulations code for performing a wide range of calculations on 3D periodic solids, 2D surfaces, gas phase clusters and isolated defects in a bulk material. In particular, GULP has a large number of materials-specific forcefields, such as the shell model for simulating ionic materials.

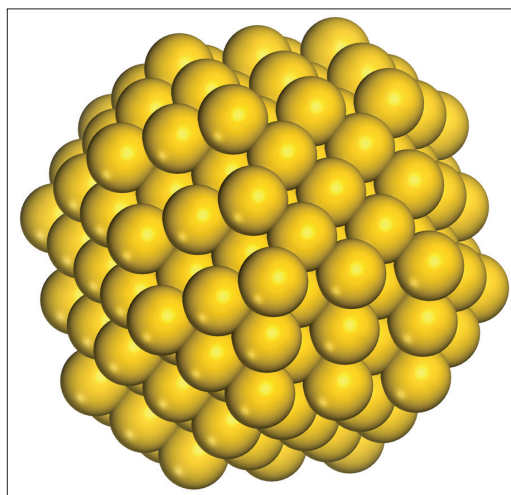
WHAT CAN GULP BE USED FOR?

GULP supports geometry optimization and molecular dynamics of molecules, clusters, and 2D and 3D systems using a wide range of potential models that span both the inorganic and organic fields. The potentials include shell model, embedded atoms (for metals), and bond order/reactive forcefields. The range of potential models means that structures as diverse as zeolites and metallic films on semiconductor substrates can be modeled.

GULP can also be used to fit and develop new forcefields with the wide range of potentials. GULP also has one of the widest range of material property analysis methods, with a particular strength in accurate vibrational analysis due to 2nd and 3rd order analytical derivatives of the potentials.

THE MATERIALS STUDIO ADVANTAGE

GULP is operated from within the Materials Studio® environment. Materials Studio provides an integrated user-interface that is easy to use and quick to learn. Materials Visualizer, the core Materials Studio product, provides all the tools you need to construct a wide range of inorganic or organic structures. Whether you need to construct a crystal cell, cleave surfaces, or build clusters and



GULP geometry optimization and dynamics can be used to study the stability of clusters such as the gold nanocluster above.

nanotubes, Materials Visualizer provides easy-to-use tools enabling you to quickly get started.

Once you have built your starting structure, you simply open the GULP interface and select the task—either single point energy, geometry optimization or molecular dynamics. Choose the potential you need and hit run. All files are transferred over to the compute server and the job is run interactively with results returned upon completion.

Integration with Materials Studio also means you can easily use other modules, such as the analysis functionality in Forcite, or a quantum mechanics module, to predict other properties.

HOW CAN GULP BENEFIT YOU?

GULP allows researchers to quickly and easily generate accurate structures and properties for a range of material types, from catalysts to fuel cells, glasses, and clays. Using GULP, you can study properties that evolve with time, as well as static properties such as Young's modulus. For a full list of properties, please see the features list.

FEATURES

System types

- Clusters, molecules and defects (0-D)
- Surfaces, slabs and grain boundaries (2-D)
- Bulk materials (3-D)
- Solvent effects can be included using the COSMO model
- An external electric field can be applied to non-periodic systems

Energy minimization

- Constant pressure / volume
- Symmetry adapted relaxation
- Unrestrained relaxation
- Constraining of internal and cell coordinates
- Newton/Raphson, conjugate gradients
- DFP or BFGS updating of the Hessian

Molecular dynamics

- NVE, NVT & NPT ensembles
- Shell model MD allowed
- Extrapolation of shells for adiabatic algorithm

Surface and attachment energies

- Calculate thermodynamic penalty for cleaving a surface from the bulk
- Calculate energy to add a stoichiometric layer of material to the surface

Libraries of potentials

Wide range of forcefield supported including:

- Organics (Dreiding)
- Zeolites and silicates (Catlow)
- Silica (Vashishta, FFSiOH)
- Carbonates
- Metal oxides (Bush, Lewis, Streitz-Mintmire)
- Glasses
- Metals (Various Embedded Atom Model libraries)
- Semiconductors (Tersoff)
- Glasses (Garofalini)
- Uranium oxide
- Valence Bond Order potential
- Reactive systems (Brenner, ReaxFF)

Crystal properties

- Elastic constants
- Bulk moduli
- Young's modulus
- Poisson's ratios
- Shear moduli
- Piezoelectric constants
- Phonon frequencies
- Non-analytic correction for gamma point modes
- Phonon densities of states
- Projected phonon densities of states
- Zero point vibrational energies
- Entropy (constant volume)
- Heat capacity (constant volume)
- Electrostatic potential
- Electric field
- Electric field gradients
- Born effective charges
- Frequency dependent dielectric constant tensor
- Optical properties (reflectivity, refractive index, dielectric constant, dielectric constant tensor)

Structure analysis

- Bond lengths, distances, angles, and torsions
- Density and cell volume
- Trajectory analysis with Forcite (license required) includes:
 - Length, angle, and dihedral analysis
 - Concentration profiles
 - Radial distribution function
 - Radius of gyration
 - X-ray scattering
 - Spatial orientation correlation function
 - Dipole autocorrelation function
 - Mean squared displacement
 - Rotational, space-time, stress, and velocity autocorrelation functions

Fitting and editing of forcefields

- Empirical fitting to elastic constants, bulk moduli, static and high frequency dielectric constants, lattice energy, piezoelectric constants, gradients, frequencies, electrostatic potential, and structure
- Simultaneous relaxation of shell positions and radii during fitting
- Relax fitting - fit to displacements rather than to gradients; this also means that the properties of the relax structures are fitted
- Fit to multiple structures simultaneously
- Vary core/shell charge split
- Vary all charges
- Wide variety of shell model, two-body, three-body, four-body, and many-body potentials available

To learn more about Materials Studio, go to accelrys.com/materials-studio