



MedeA *MLProperty*

From representation to properties

At-a-Glance

The MedeA^{®1} *MLProperty* tool enables rapid calculation of atomic-scale properties using their machine-learned representations generated from first-principles calculations. Building on *MedeA Machine-Learned Potential* representations, it provides efficient access to partial electronic charges, core level energies, electric field gradients, and partial electronic density of states (DOS).

Key Benefits

Efficiency

- Rapid property calculations on structures or structure lists
- Direct integration into MedeA flowchart workflows
- Uses machine-learned representations stored in *.frc* format

Versatility

- Batch processing of structure ensembles
- Systematic property screening capabilities

Accuracy

- Founded on rigorous first-principles reference data
- Results comparable to direct first-principles calculations

file, partial electronic charges, core level energies, electric field gradients, and partial electronic DOS are computed and provided as tabular or graphical output.

Partial Electronic Charges

Atomic charges relate to electron density and can be inferred from first-principles calculations, though no unique assignment scheme exists. Common approaches include representations of the wave function (Mulliken, Löwdin), electronic density (Bader, Hirschfeld), electrostatic potential (ESP), or polarization charges (Born effective charges).

Core Level Energies

The calculations of partial electronic charges are complemented by calculations of another scalar property, namely, the energy of core levels. The results obtained from both MedeA VASP and the GRACE machine-learned representation are directly comparable, enabling validation and refinement of machine-learned models across diverse chemical systems and structures.

Electric Field Gradients

Electric field gradient (EFG) tensors characterize the anisotropy of the charge density in the vicinity of atomic nuclei. These tensors are symmetric and therefore contain six independent components. The theoretically predicted values can be compared to experimental data measured by spectroscopic methods (Mößbauer, Perturbed Angular Correlation (PAC), Nuclear Quadrupole Resonance (NQR), Nuclear Magnetic Resonance (NMR), and muon Spin Rotation (μ SR)) since the quadrupolar nuclear moment interacts with the EFG resulting in hyperfine splitting. The sensitivity to details of the electronic charge distribution makes the EFG a powerful tool for the investigation of the chemical environment of the nucleus.

Atomic-Scale Property Calculations

Atomic Properties from Machine-Learned Representations

The *MLProperty* tool is invoked within the MedeA flowchart paradigm to calculate properties for given structures or structure lists. After reading the machine-learned representation from an *.frc*

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Partial Electronic Density of States

Electronic density of states (DOS) characterizes the spectrum of energy levels in a system. Evaluation of partial electronic densities requires definition of the integration sphere. Semi-core states may be included in pseudopotentials to increase accuracy, appearing as narrow peaks ~10 eV below the Fermi energy. For DOS fitting, semi-core states can be removed, though they assist in aligning DOS curves to a common energy scale—a necessary step since electrostatic potential values shift differently across calculations.

Implementation in *MedeA*

DOS transformation to Chebyshev moments before fitting and back-transformation by *MLProperty* automates pre- and post-processing. The graphical user interface allows control of the number of Chebyshev moments, providing flexibility between accuracy and computational efficiency.

Technical Features

Property Calculations

- Partial electronic charges
- Core level energies
- Electric field gradients
- Partial electronic density of states (DOS)

Integration and Workflow

- *MedeA* flowchart integration
- Batch processing of structure ensembles
- Direct import of *MLProperty* machine-learned representations (.frc files)
- Graphical and tabular output

Key Features

- Uses machine-learned representations generated from *MedeA Machine-Learned Potential Generator*
- Rapid property evaluation compared to first-principles calculations
- Systematic property screening capabilities
- Full *MedeA* environment integration

Required Modules

- *MedeA Environment*
- *MedeA ML Property*
- *MedeA Machine-Learned Potential Generator*
- *MedeA Machine-Learned Potential*

Related Modules

- *MedeA VASP*

