MedeA MT

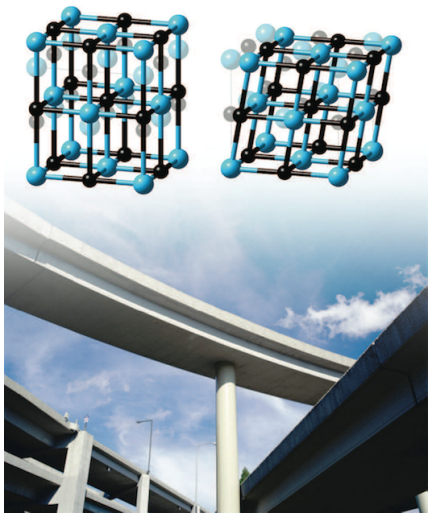
Explore Elastic Response and Mechanical Stability of Materials

At-a-Glance

MedeA®[1] *MT* highly efficiently and effectively calculates key mechanical and thermodynamic properties of metals, semiconductors, ceramics, glasses, polymers, and thermosets.

Key Benefits

- Fully automated and robust computational procedure, designed to achieve utmost accuracy for the elastic coefficients as compared to other available approaches
- Automatic prediction of a wealth of derived, technologically important data, such as stability analysis, polycrystalline moduli, descriptors for hardness and ductility, Debye temperature, and estimates for the thermodynamic functions
- Statistically rational results, especially for polymers, thermosets, and amorphous systems
- Straightforward combination of different computational approaches in a single workflow



By means of a fully automated procedure evaluating the elastic response to lattice distortions[2], *MedeA MT* calculates mechanical and thermodynamic properties of crystalline, polycrystalline, and amorphous materials. Especially, for amorphous materials *MedeA MT* precisely and quantitatively predicts elastic properties by means of statistical sampling within the Hill-Walpole approach, as improved by Suter and Eichinger.[3]

'The symmetry generality of the approach described here enabled the creation of a robust user interface going seamlessly from the database search to the printout of the elastic coefficients. With it, even non-specialist users can reliably produce technologically relevant results. . . '

Yvon LePage and Paul Saxe (abstract of [2])

Properties from *MedeA MT*

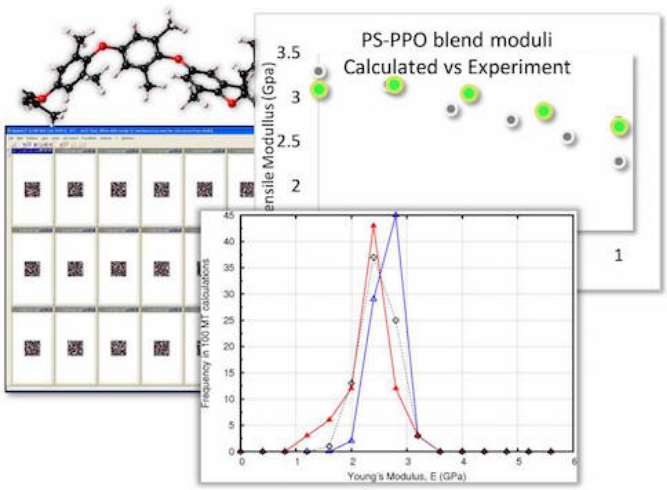
- Elastic coefficients with estimation of numerical uncertainty
- Mechanical stability analysis, using the eigenvalues of the elastic coefficient matrix
- Elastic moduli (bulk, shear, and Young's moduli) from polycrystalline averaging (Voigt, Reuss, and Hill)
- Precise bounds estimate for elastic properties of polymers and glasses
- Poisson's ratio, Pugh's ratio, and Vickers hardness as descriptors for Poisson effect, ductility, and hardness
- Velocity of sound
- Debye temperature
- Temperature dependent thermodynamic functions calculated within the Debye model
  - Heat capacity

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] Y. LePage and P. Saxe, *Physical Review B* **65**, 104104 (2002)

[3] U. W. Suter and B. E. Eichinger, *Polymer* **43**, 575 (2002)

  - Zero-point energy
  - Vibrational enthalpy, entropy, and free energy
- Temperature dependent thermal expansion coefficient estimated from Debye-Grüneisen approach



Computational Characteristics

- Predicts key mechanical properties within the elastic regime
- Automatic detection and use of any space-group symmetry
- Iterative full relaxation of all atomic degrees of freedom of distorted structures resulting in utmost accuracy (as compared to exploiting the Hessian only once)
- Supported compute engines for optimization and stress tensor evaluation
  - *MedeA VASP* – recommended for metals, semiconductors, ceramics, and molecular crystals
  - *MedeA LAMMPS* – recommended for polymers and thermosets, and amorphous materials
  - *MedeA MOPAC* – recommended for molecular crystals
- Determination of minimum set of elastic coefficients, compliances, and their matrices
- Configurational sampling and improved Hill-Walpole bounds analysis for polymers, thermosets, and amorphous systems
- Exhaustive use of methods available in *MedeA VASP*, such as LDA, GGA, GGA+U, meta-GGA, van der Waals, and hybrid functionals, spin-polarization, and fully relativistic Hamiltonians
- Fully automated setup, execution, and processing of calculations with any of the recommended compute engines
- Restart capabilities in case of hardware or any other failures

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA VASP* (required for ab-initio prediction of mechanical and thermal properties)
- *MedeA HT-Launchpad* (required for Hill-Wallpole sampling)
- *MedeA HT-Descriptor*
- *MedeA Amorphous Materials Builder* (required for polymers, thermosets and amorphous materials)
- *MedeA Pearson*

Tightly Integrated Modules

- *MedeA EAM*
- *MedeA MOPAC*

Find Out More

Watch the Webinar: Predicting Elastic Properties Using Ab Initio and Forcefield Based Simulations

Learn how to calculate elastic constants with *MedeA VASP 5* and *MedeA LAMMPS* in these tutorials:

- How to Calculate Elastic Constants with MedeA VASP 5
- How to Calculate Elastic Constants with LAMMPS

Applications of *MedeA MT* are demonstrated in the following Materials Design Application Notes:

- Stability of Alkaline-Earth Hydrides
- Elastic coefficients and moduli for silicon carbide (β -SiC), corundum (α-Al_2O_3\), and ferric tourmaline (schörl)

- Change of Elastic Properties of Graphite Electrode upon Li Intercalation

- Effect of Resin Molecular Architecture on Epoxy Thermoset Mechanical Properties

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