materials design

MedeA MT: Examine Materials Mechanical Stability

Materials Design builds bridges that connect problems to solutions. Our MedeA MT module efficiently calculates mechanical and thermodynamic properties of both crystalline and polycrystalline materials.

Key Benefits of MT:

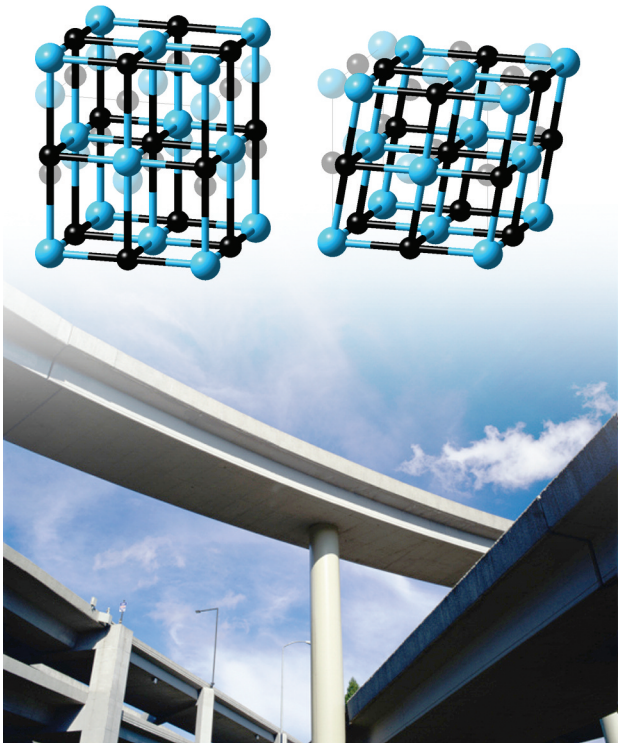
- *Predicts key mechanical properties*
- *Performs mechanical stability analysis*
- *Estimation of thermodynamic properties at finite temperatures*

Properties from MT module:

- *Elastic coefficients (in GPa) with estimation of numerical uncertainty*
- *Stability analysis of crystals through the eigenvalues of the elastic coefficient matrix*
- *Bulk, shear, and Young's modulus with polycrystalline averaging (Voigt, Reuss, Hill)*
- *Velocity of sound*
- *Debye temperature*
- *Temperature dependent heat capacity within Debye model*
- *Estimation of vibrational enthalpy, entropy, free energy, and zero-point energy and thermal expansion coefficients*

Computational characteristics:

- *Calculates stress tensors for strain-reduced symmetries by re-optimization*
- *More accurate elastic constants than by simple stress estimates with VASP standalone*
- *Automatic detection and use of any space-group symmetry*
- *Determination of minimum set of elastic coefficients*
- *Fully automated setup, execution, and processing of VASP jobs*
- *Uses stress tensor computed with VASP 4.6 or 5.2 with any of the functionals available. This includes the ability to use functionals such as GGA+U and hybrid functionals, and fully relativistic Hamiltonians*
- *Restart capabilities in case of hardware or communication failures*



Required MedeA modules:

- *Core MedeA environment*
- *MedeA VASP 4.6 or 5.2*
- *MedeA MT*
- *JobServer and TaskServers*

More on our website:

- ***MedeA MT in Depth: Forsterite Mg_2SiO_4***
- ***Elastic coefficients and moduli for cubic silicon carbide (β-SiC), corundum (α-Al_2O_3), and a tourmaline crystal (Schorl)***
- ***Alkaline-earth hydrides***
- ***Graphite Electrode Elastic Properties upon Li Intercalation***

*Visit our website **www.materialsdesign.com** or contact your local Materials Design office for further information.*

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