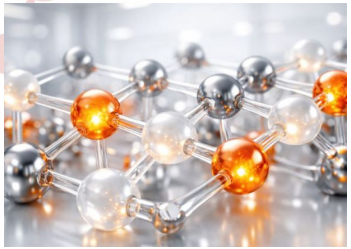
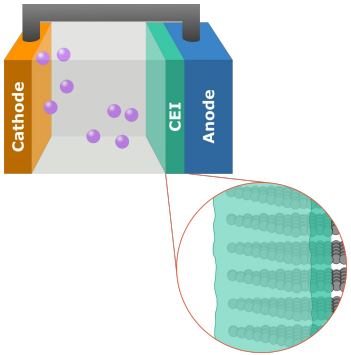
Predictive Modeling for Component Robustness

Predicting Material Failure and Endurance via Quantum Mechanical Properties





The Challenge:

Novel material often **lack the precise mechanical properties** required for engineering models

The Solution:

Virtually "stress test" materials at the atomic level. Extracts **critical constants;**

- **Young's Modulus** for stiffness
- **Shear Modulus** for shape resistance

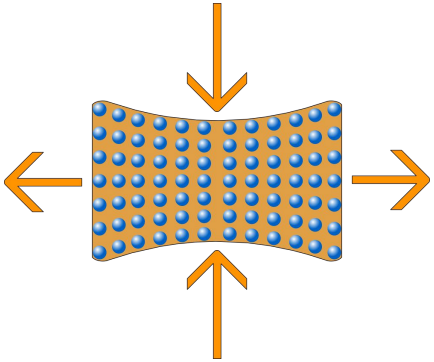
Strategic Impact:

- **Accelerated R&D**
- **Reliable CAE Input**
- **Enables digital "screening"**

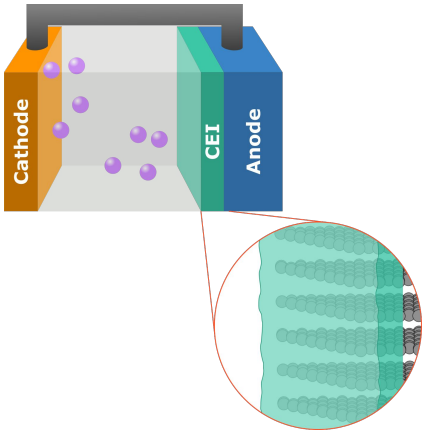
The Challenge

Many industries (automotive, chemistry, energy) require **knowing material deformation** and **failure processes**.

New material designs lack necessary constants (elasticity, strength) to predict performance in engineering applications.



Example: In Li-ion batteries, knowing the mechanical properties of the Solid Electrolyte Interphase (SEI) is crucial to predict expansion/cracking and ensure battery lifetime.



The Solution: Quantum Elasticity Mapping

ASAP (Atomistic Simulation Advanced Platform)

ASAP utilizes Density Functional Theory (DFT) methodology (SIESTA and Quantum Espresso codes) to accurately predict the mechanical response of new materials by simulating the effect of strain on the atomic structure.

Characteristics computed:

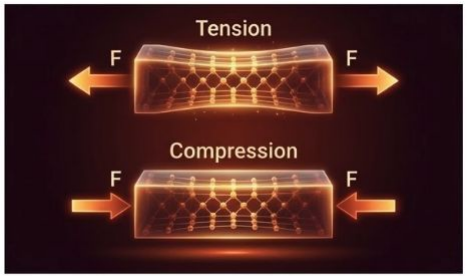
- Stress Tensor and Elastic Constants

ASAP calculates the stress tensor induced by an applied strain. The Elastic Constants (C_{ij}) are subsequently derived from these quantum-mechanical results, providing the foundational material properties for engineering models: **Young's modulus** (E_R) and **Shear modulus** (G_R).

Core Insight: Quantum Elasticity Mapping

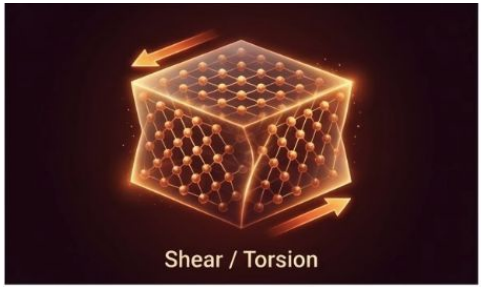
Young's modulus (E_R) Stiffness/Rigidity

Measures the material's resistance to elastic deformation (stretching or compression) under tensile stress. This is the most fundamental indicator of a structural component stiffness under load.



Shear modulus (G_R) Shape Resistance

Measures the material's resistance to shearing force or torsional (twisting) stress. This is crucial for understanding how a material resists internal failure and deformation before cracking

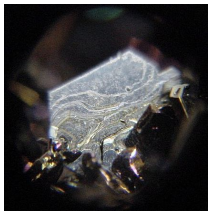


They are the essential material constants required to feed into macro-scale Computer-Assisted Engineering (CAE) methods used for component design.

Impact: Digital Material Qualification

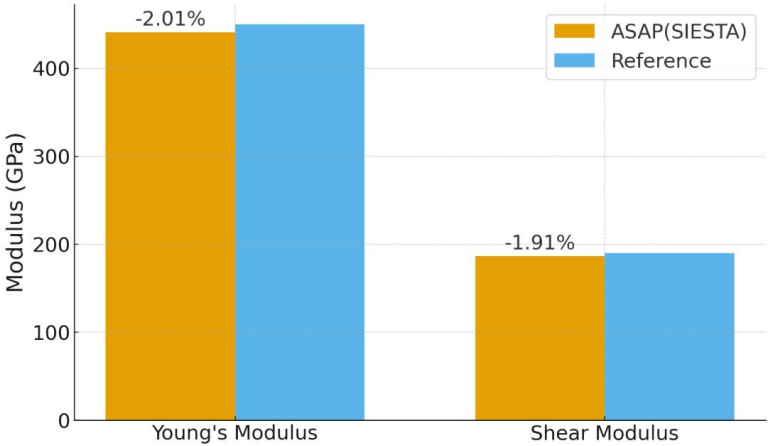
- **Accelerated Engineering:** Provides robust material constants for new and innovative materials that cannot be measured experimentally yet.
- **Reliable CAE Input:** Delivers the required material constants to feed into macro-scale Computer-Assisted Engineering (CAE) methods used in automotive, aviation, and shipbuilding.
- **Risk Reduction:** Enables digital testing of novel materials, avoiding physical experiments and validating robustness before prototyping

Technical Validation: Hard Ceramics



Silicon Carbide (SiC) is widely used in applications requiring high endurance, such as car brakes, car clutches, plates in bulletproof vests.

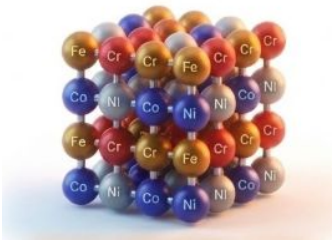
ASAP accurately predicts the elastic constants for SiC, demonstrating a maximum deviation of only -2.01% from the reference values, **validating** the ability to **model hard ceramics**



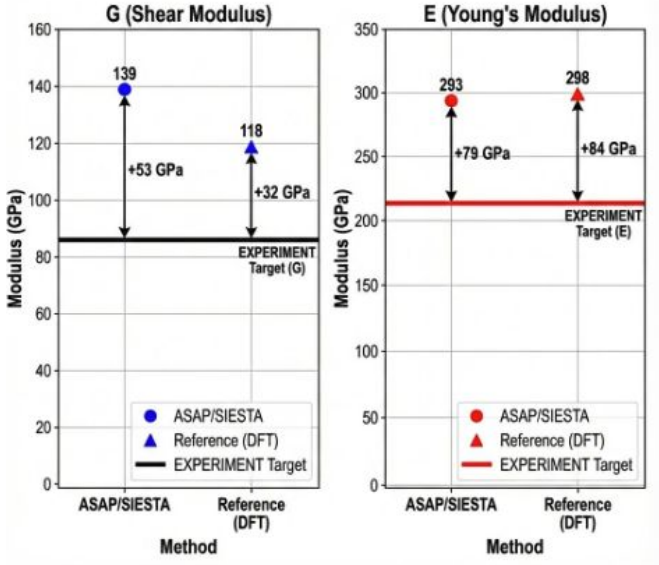
Reference
https://next-gen.materialsproject.org/materials/mp-806

Technical Validation: Complex Metallic Alloys

High-Entropy Alloys (HEA), are used as advanced structural components used in high-stress, high-temperature environments (e.g., gas turbines or nuclear reactor components). Successfully modeling of HEA is key for predicting long-term endurance and mechanical stability.



ASAP/SIESTA calculations achieve predictive accuracy comparable to industry-standard reference* DFT method establishing a robust baseline for predicting endurance in HEA



Reference (DFT-VASP): N. Koval, J.I. Juaristi, R.M. Muino, M. Alducin, J. Appl. Phys. 127, 145102 (2020); https://doi.org/10.1063/1.5142239

Technical Validation: Publications

These publications validate the DFT methodology. ASAP automates the required calculations for rapid R&D application.

- Some Principles of Strength Designing for Turbine-Blade Protective Coatings
- On the Electronic, Mechanical and Optical Properties of Superhard Cross-Linked Carbon Nanotubes (Tubulanes)
- Numerical Evaluation of the Elastic Moduli of AlN and GaN Nanosheets
- Determination of Structural, Electronic, and Elastic Properties of $SnTiO_3$

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