An EMTO database of elastic constants for pure elements

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The elastic constant tensor, along with the volume and the bulk modulus, is fundamental to the understanding of mechanical properties of materials. Elastic constants provide insight into the bonding in the material and they also correlate with many macroscopic mechanical properties, such as ductility, brittleness, and hardness. In this light, it is interesting to note that only a couple of systematically computed elastic constant databases have been reported [1,2] and they are both limited to the same computational method (projector-augmented wave method as implemented in VASP).
To compare different computational methods and to verify the results of the previous databases, we have calculated the elastic constants of a large set of pure elements using the exact muffin-tin orbitals method (EMTO). Elastic constants of pure elements are often needed when modeling multicomponent systems e.g. through the CALPHAD approach. To handle the large workload, modern many-task computing and automation approaches [2-5] have been utilized. This database will form a part of the basis for future projects, such as modeling and understanding high-entropy alloys and other multicomponent systems.

References

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