MAR15-2014-020250

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Distributed databases for materials study of thermo-kinetic properties

CORMAC TOHER, Duke Univ

High-throughput computational materials science provides researchers with the opportunity to rapidly generate large databases of materials properties. To rapidly add thermal properties to the AFLOWLIB consortium [1, 2, 3, 4] and Materials Project repositories [5], we have implemented an automated quasi-harmonic Debye model, the Automatic GIBBS Library (AGL) [6, 7]. This enables us to screen thousands of materials for thermal conductivity, bulk modulus, thermal expansion and related properties. The search and sort functions of the online database can then be used to identify suitable materials for more in-depth study using more precise computational or experimental techniques. AFLOW-AGL source code is public domain and will soon be released within the GNU-GPL license.

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