The self-referential method for calculating crystal free energies

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A new method for calculating crystal free energies that is particularly straightforward is described. This self-referential method calculates the difference in free energy between large (double-size) and small (single-size) crystal systems using two stages; the replication stage is analytic while the relaxation stage is performed efficiently using a kind of thermodynamic integration. Results are presented for several reasonably simple crystals. It is also shown how this self-referential method can be applied to more complex crystals and crystals in confined geometries.