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CLUSTER POTENTIALS FROM EXACT INVERSION OF AB INITIO ENERGY DATA,
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Carlsson et.al. have shown that ab initio cohesive energy vs. volume curves can be inverted to obtain radial pair potentials that reproduce the data.[1] Their proof relies on expressing the energy as a sum of linear operations on the radial pair pair potential. By generalizing an alternate proof involving recursions that do not rely on linearity, it is possible, given assumed angular dependencies, to obtain all radial factors in many-body cluster expansions that reproduce a set of cohesive energy curves. One data curve is needed for each radial function, but, if additional curves are used, the equations are overdetermined and inconsistent, because the assumed angular form is never perfect. The consistency of the radial functions obtained by inverting multiple data sets, however, provides a quantitative measure of how well the functional form of the angular factor (not the just parameters) models the bonding preferences of the material in various environments. Such capability can guide the development of potentials for covelently bonded materials. The application of our formulas to silicon energy data demonstrates how an analytic tool for evaluating proposed functional forms is a useful supplement to the usual simulated annealing fit of potential parameters.

[1] A.E. Carlsson, C.D. Gelatt,Jr. and H. Ehrenreich, *Phil. Mag. A*, **41**, 241-250 (1980).

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