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Ising-like Description of Structurally Relaxed Ordered and Disordered Alloys

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We demonstrate the ability of generalized Ising-like cluster expansions to describe the energetics and thermodynamics associated with large atomic displacements in alloys. Although the expansion is constructed only from the energies of a few (small-unit-cell) ordered structures, it provides

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0.8 0.6 0.4

LRO parameter, q

0.2 0.0

FIG. 3. Formation energies of Ga05lno5P alloys as a function of LRO parameter, g. Directly calculated results from 1000-atom simulations are shown as are the results of the k-space CE, using as input only rl = 1 energies. rl = 1 (0) indicates complete and perfect order (randomness).

composition-temperature phase diagram (open squares of Fig. 4). Here we apply the Monte Carlo algorithm to DHOLE[(5;)] with only spin degrees of freedom, finding the CE prediction for the phase diagram (solid line in Fig. 4). The phase diagram computed using unrelaxed

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