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Orientational ordering of tetrahedral clusters in $CaCd_6$ alloy WOOSONG CHOI, Cornell University, MAREK MIHALKOVIC, Slovak Academy of Sciences, CHRIS HENLEY, Cornell University — In icosahedral CaCd quasicrystals and related alloy structures, each icosahedral cluster contains an innermost tetrahedral shell that is loosely coupled with its shell. We extract an effective potential for the pair interaction $V(\Omega, \Omega')$ of the orientations Ω of neighboring clusters, as mediated by the intervening atoms. Using the EAM potentials of Brommer et al., [1]we relax all atoms, with each tetrahedron constrained to a chosen (continuously variable) overall orientation but allowing distortions. Using singular value decomposition, the relaxed energies are represented as $V(\Omega, \Omega') = \sum_j A_j f_j(\Omega) f'_j(\Omega')$ where only a few terms are important and the f_j's have simple sinusoidal forms (which can be understood physically). We thus obtain a fit with only a few parameters, in place of the 46-parameter fit of Brommer et al[1] based on 12 discrete orientations. By Monte Carlo simulations with the obtained interaction, we determine the pattern of the orientationally ordered state seen experimentally below $\sim$ 90K, and check the ordering transition previously simulated only in small system sizes[1].

[1]Brommer, Gähler, and Mihalkovič, Phil. Mag. 87, 2671 (2007)

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