PHYSICAL REVIEW B VOLUME 45, NUMBER 5 1 FEBRUARY 1992-I

First-principles calculation of the order-disorder transition in chalcopyrite semiconductors

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(Received 23 September 1991)

We describe the polymorphic order-disorder transition in the chalcopyrite-type semiconductor
Cuo.slnosSe through a Monte Carlo simulation of a generalized Ising Hamiltonian whose interaction
energies are determined from ab initio total-energy calculations. The calculated transition tempera-ture (T, =1 l25+'20 K) compares well with experiment (T, =1083 K). Unlike the analogous ordering in isovalent III-V alloys, we find that the transition is dominated by

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TABLE I. LAPW calculated relaxed excess energies [Eq.
(I)] of Cuo~lno~Se in various structures defined in the text. Fit-
ting these io Eq. (3) using six interaction energies (see text)