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New insights into the electronic properties of ordered semiconductor alloys: non-parabolic and non-analytic dependence on the order parameter YONG ZHANG, UNC-Charlotte, A. MASCARENHAS, S.-H. WEI, NREL, L.-W. WANG, LBL — It is both fundamentally and practically important to understand the dependence of a physical property on order parameter η for an ordered semiconductor alloy like $Ga_xIn_{1-x}P$ that is often found to be in a partially ordered phase. A conventional statistical theory based on a cluster expansion approach predicts that for any physical property P(x,η) the leading term of the dependence is η^2 with higher order corrections $\eta^4$and etc., thus, always an analytic function of η^2. From the practical application point of view, it is highly desirable to see that the η^2term, corresponding to the pair correlation, alone can give adequate accuracy. However, we have found that for the electronic structure not only η^2term is often inadequate but also non-analytic dependence on η^2may sometimes arise, depending on the strength of the coupling among virtual crystal states caused by the alloying and ordering.[1] The predictions have been confirmed experimentally.[2] The results provide *a priori* principle about the applicability of the conventional cluster expansion method to the description of the electronic structure of the semiconductor alloy, and a general understanding of the order parameter dependence of an electronic property in a semiconductor alloy. [1]Zhang et al, PRB80,045206(09). [2] Steiner et al, JAP106,063525(09). DOE/BES

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