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 $\eta$ for an ordered semiconductor alloy like Ga$_x$In$_{1-x}$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 $P(x,\eta)$ the leading term of the dependence is $\eta^2$ with higher order corrections $\eta^4$ and etc., thus, always an analytic function of $\eta^2$. From the practical application point of view, it is highly desirable to see that the $\eta^2$ term, corresponding to the pair correlation, alone can give adequate accuracy. However, we have found that for the electronic structure not only $\eta^2$ term is often inadequate but also non-analytic dependence on $\eta^2$ may 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