First-Principles Combinatorial Design of Transition Temperatures in Multicomponent Systems: The Case of Mn in GaAs

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The transition temperature T_C of multicomponent systems—ferromagnetic, superconducting, or ferroelectric—depends strongly on the atomic arrangement, but an exhaustive search of all configurations for those that optimize T_C is difficult, due to the astronomically large number of possibilities. Here we address this problem by parametrizing the T_C of a set of ~50 input configurations, calculated from first principles, in terms of configuration variables (‘‘cluster expansion’’‘6

stant of the solids exhibiting these phenomena. The quest for materials with desired T_C’s, such as high-temperature superconductors or room-temperature ferromagnetic semiconductors, characterizes much of contemporary materials science. The ability to intentionally grow in the laboratory different structural realizations of substitutional alloys, even in defiance of thermodynamical equilibrium, has opened up the challenging prospect of attaining special T_C’s by manipulating the growth parameters. Indeed, the realization that transition temperatures can be controlled by alloying two or more component materials has spurred considerable interest in materials engineering of metal alloys [1], multicomponent superconducting alloys [4], ferromagnetic semiconductors alloys made of both magnetic and nonmagnetic components [2], ferroelectric alloys [3], etc. Interestingly, the transition temperature of the combined, multicomponent system rarely follows a constituent-average, linear behavior. Instead, T_C is often determined by the *a a a* in the system. Numerous attempts [5,6] have already been made to grow $Ga_{1-x}Mn_x$

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structures represent a range of Mn concentrations and layer orientations. We then use the calculated $\{T_C^{\mathrm{LDA}}(\quad_{\mathrm{input}})\}$ to determine the coefficients of Eq. (1). We include in the ture of the random alloy can be exceeded by growing digital heterostructures on currently unsuspected substrate orientations. Since it is often easier to grow