

# First-Principles Combinatorial Design of Transition Temperatures in Multicomponent Congurations, Causing Expansion of the Solid Exhibiting these Phenomena. The Quest

$T_C$ '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 semiconductor 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  $a$ ,  $a$ ,  $a$ ,  $a$  in the system. Numerous attempts [5,6] have already been made to grow  $\text{Ga}_{1-x}\text{Mn}_x$

(.) Ca  $\dots$  a  $\dots$  a  $\dots$  a  $\dots$   
a  $\dots$  a  $\dots$

structures represent a range of Mn concentrations and layer orientations. We then use the calculated  $\{T_C^{\text{LDA}}(\text{input})\}$  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