# Computational Nano-Materials Design for Semiconductor Nanospintronics: Spinodal Nano-decomposition, Codoping, and New Materials

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We will summarizes the recent progress on computational nano-materials design, experimental realization and control methods of spinodal nano-decomposition under the three- and two dimensional crystal-growth conditions in spintronic materials such as dilute magnetic semiconductors (DMS). We review the computational simulation of nano-spinodal decomposition by combining first-principles calculations and kinetic Monte Carlo simulations. Via simulations of the spinodal decomposition in various systems, such as (Ga,Mn)N, (Zn,Cr)Te, (Zn,Co)O. We point out that the spinodal nanodecomposition can be generalized as a new class of bottom-up nanotechnology with an outstanding potential in various fields.

Based on first-principles calculations and kinetic Monte Carlo simulations, we design a realistic and practical codoping technique for increasing the concentration of Mn atoms in GaAs and realizing high Curie temperatures ($T_C$) in (Ga,Mn)As. We found that using codoping of Li interstitial atoms during the crystal growth has two great advantages. First, due to lower formation energy of Li interstitials compared to Mn interstitials, Li prevents formation of unwanted Mn interstitials. Second, Li interstitials can be removed by using post-growth annealing at low temperatures. This codoping method offers a general strategy to go far beyond the solubility limit and it should be applicable also to other diluted magnetic semiconductor systems.

The electronic structure and the magnetic properties of Mn-doped GeTe are calculated from first-principles. It is shown that Mn-3*d* states appear deep in the valence bands with $d^5$ electron configuration and the system is insulating. By introducing Ge vacancies to dope hole carriers, the ferromagnetism is induced via the *p-d* exchange mechanism. The electronic structures of Mn-doped LiZnAs, LiZnP and LiZnN are calculated. Firstly, by estimating free energy, phase diagrams of these systems are predicted. It is shown that these systems are phase separating systems and favor spinodal decomposition. However, by introducing Li vacancies, spinodal decomposition is strongly suppressed and Mn can be doped up to high concentration. Moreover, the introduced Li vacancies induce ferromagnetic interaction between Mn and thus we can expect high $T_C$ in these systems. To see the chemical trend, electronic structure and $T_C$ of Li(Zn, Cr)As are also calculated.

We present a first-principles study of the magnetic properties of N-doped MgO, CaO and SrO, which have been proposed to constitute a new class of DMS with no magnetic elements. In this study, it was found that under a homogeneously distributed condition, Tc could reach room temperature at sufficient N concentrations in the range of 20 to 30 at.%; however, an inhomogeneous N distribution in these DMSs is the favored configuration, which indicates that spinodal decomposition leads to a room-temperature blocking temperature at smaller N concentrations than those estimated for room-temperature ferromagnetism in the homogeneous distribution condition.