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Codoping of (Ga,Mn)As as a route to higher $\mathbf{T}_c$ LARS BERGQVIST, Dept. of Physics, Uppsala University, KAZUNORI SATO, Graduate School of Engineering Science, PETER DEDERICHS, Forschungzentrum Julich, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science — We will present a theoretical study of diluted magnetic semiconductors (DMS) with focus on (Ga,Mn)As. Earlier studies have revealed that the critical temperatures should rapidly increase with Mn concentration and could potentially reach room temperature if no compensating defects are present. Using Li interstitial atoms as codoping elements in (Ga,Mn)As, we have found a promising way to boost the Mn concentration to large values (> 20 %). However, the Li interstitials destroy the ferromagnetic properties of (Ga,Mn)As and in order to have a functional material, the Li atoms needs to be removed from the system using annealing techniques, similar to what is used to remove Mn interstitials. Therefore we have performed a detailed study of the diffusion dynamics such as migration barriers etc of Li interstitials using very large scale supercell calculations employing special quasirandom structures and compare this with the case of Mn interstitials. Moreover, several defect complexes consisting of Li (Mn) interstitials and Mn substitutionals have been considered. It is found that the migration barrier for a Li interstitial is typically lower than for a Mn interstitial, however the migration barrier for the latter case is very dependent on local environment effects.

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