

Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky, Yousef Saad and Renata Wentzcovitch (Minnesota), Steven G. Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR-0325218): Growth of Mn on Ge Surfaces

Understanding growth mechanisms of spintronics materials such as Mn:Ge is an important, but largely unexplored issue. We use pseudopotential-density functional theory to examine the growth of Mn on Ge surfaces. We find that low Mn doses on Ge (100) surface initiates novel subsurface growth whereas Mn on the (111) surface can diffuse into the bulk via interstitial sites. On the right, we show various positions of Mn on the (100) Ge surface. All the sites are less energetically favorable than the interstitial site (I_0). As such, thermodynamic considerations suggest that Mn will always reside just beneath the Ge surface.

