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The onset of Mn monomer and dimer adsorptions on GaAs(110)[1]
JUE-XIAN CAO, ICTS, Beijing, China, XIN-GAO GONG, Fudan University, China, LU YU, ICTS, Beijing, China, RUQIAN WU, UC Irvine — Using the density functional VASP and FLAPW approaches, we studied the onset of Mn adsorption on GaAs(110). Large unit cells were used to explore the limit of monomer and dimer adsorbates. We found strong interplay between the magnetization and adsorption geometry, including substitution of Mn on the surface Ga sites. For Mn dimers, the nearest Mn-Mn distance is 8.1 Å, a result which agrees with recent STM observations. These results are explained from electronic structures and lay a basis for further understanding of the mechanism of growth and magnetic ordering in(Ga,Mn)As, a prototype dilute magnetic semiconductor for spintronics applications.

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