

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

The structural, electronic and magnetic properties of Ga $_{8-x}$ Mn $_x$ As $_8$ clusters¹ GANGXU GU, GANG XIANG, College of Physical Science and Technology, Sichuan University — We systematically investigate the ground-state magnetic properties of Ga $_{8-x}$ Mn $_x$ As $_8$ clusters ($x = 0, 2, 4, 6,$ and 8) within the framework of density functional theory (DFT) using a strategy that successively adopts the particle swarm optimization (CALYPSO) code and fixed spin-moment (FSM) method. The results show that for Ga $_{8-x}$ Mn $_x$ As $_8$ in the ground states or low-lying isomers, Mn atoms tend to assemble at the core of the clusters and the ferromagnetic Mn-Mn couplings are identified for Ga $_{8-x}$ Mn $_x$ As $_8$ ($x=4, 6,$ and 8), while Ga $_8$ As $_8$ and Ga $_6$ Mn $_2$ As $_8$ are nonmagnetic. The possibility of multiple ground states of Ga $_{8-x}$ Mn $_x$ As $_8$ ($x = 4, 6,$ and 8) is also demonstrated. The binding energy and LUMO-HOMO gap analysis show that Ga $_{8-x}$ Mn $_x$ As $_8$ clusters with large x are more likely synthesized and exhibit stronger chemical reactivity.

¹the Natural Science Foundation of China (NSFC) Grant No. 11174212

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Date submitted: 12 Nov 2014

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