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**Theoretical studies of the magnetic properties of Mn trimers on the (110) GaAs surface** FHOKRUL ISLAM, Linnaeus University, REZA MAHANI, KTH, Royal Institute of Technology, DAVIDE GROSSI, PAUL KOENRAAD, Technische Universiteit Eindhoven, CARLO CANALI, Linnaeus University — Transition-metal impurity-doped GaAs has been the most intensively studied prototypical model system for understanding the magnetic properties of dilute magnetic semiconductors (DMS). While the study of isolated pairs of impurity provides insight about the nature of magnetic interactions in DMS, addressing larger clusters of magnetic impurities is essential for realizing complex magnetic phenomena such as spin frustration, spin-electric coupling and spin waves, which can be used in quantum information storage and processing. In this work, motivated in part by ongoing scanning tunneling spectroscopy (STM) experiments, we have investigated theoretically the electronics and magnetic properties of different Mn trimer configurations on the (110) surface of GaAs, using first-principles density functional theory (DFT) and microscopic tight-binding (TB) methods. We have employed DFT to study the physical stability and magnetic ground states for both collinear and triangular trimers and their dependence on crystallographic axes. The TB calculations, carried for some of the most stable Mn trimer configurations on the GaAs surface, yield information on the electronic structure and the local density of states associated with the Mn acceptor holes, which is directly probed in STM measurements.

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