

Abstract Submitted
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Digital Ferromagnetic Heterostructure Composed of Mn in Si¹

C. Y. FONG, M. C. QIAN, UC Davis — We examine the electronic and magnetic properties of digital ferromagnetic heterostructures (DFH) composed of Mn atoms confined in a layer of Si by using an *ab-initio* algorithm. The δ -layer can have the composition of $\text{Mn}_{1-x}\text{Si}_x$ with $x=0$ for 1ML, $x=0.5$ for 0.5ML, and $x=0.75$ for 0.25ML coverage of Mn. Each DFH is simulated by a tetragonal supercell formed by stacking 8 cubes of the Si crystal in the [100] direction. For each supercell, the value of x determines the area of the plane perpendicular to the [100] direction. For all cases, the total energy difference between the ferro- and antiferro-magnetic phases, the magnetic moments for the ferromagnetic phase, and the density of states at the Fermi energy as functions of x will be presented.

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