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A theoretical study of volume-dependent exchange interactions in MnAs BIPLAB SANYAL, CAMILLE ARON, OLLE ERIKSSON, Department of Physics, Uppsala University, Sweden — We have studied magnetic interactions in zinc-blende MnAs as a function of volume by *ab-initio* density functional calculations. The calculated Heisenberg pair-exchange parameters show a strong volume dependence. The calculated Curie temperatures, obtained from by Monte-Carlo simulations using *ab-initio* parameters and a classical Heisenberg Hamiltonian, show a decreasing trend upon compression. Analysis of cross-sections of Fermi surfaces indicate a nesting feature for compressed volumes, which can give rise to competing exchange interactions. Calculations of self-consistent noncollinear spin configurations indicate that spins deviate strongly from collinear ordering for low volumes whereas they align in a collinear ferromagnetic fashion for high volumes. Also, for expanded volumes, the calculated Curie temperature is around 600 K signifying the possibility of using MnAs for future room-temperature spintronic applications.

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