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Proposed Orbital Ordering in MnV_2O_4 from First-principles Calculations[1] TANUSRI SAHA-DASGUPTA, SOUMYAJIT SARKAR, S.N.Bose National Centre for Basic Sciences, TULIKA MAITRA, Department of Physics, Indian Institute of Technology, Roorkee, India, ROSER VALENTI, Institut für Theoretische Physik, J. W. Goethe Universität, Frankfurt, Germany — Based on density functional calculations, we propose a possible orbital ordering in MnV_2O_4 which consists of orbital chains running along crystallographic a and b directions with orbitals rotated alternatively by about 45° within each chain. We show that the consideration of correlation effects as implemented in the local spin density approximation (LSDA)+U approach is crucial for a correct description of the space group symmetry signifying a strong influence of the correlation-driven orbital ordering on the structural transitions in this system. Inclusion of spin-orbit effects does not seem to influence the orbital ordering pattern. We further find that the proposed orbital arrangement favors a non-collinear magnetic ordering of V spins, as observed experimentally. Exchange couplings among V spins are also calculated and discussed.

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