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Study of band width narrowing/broadening in monatomic chains

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Gamberdella et al. demonstrated the first controlled realization of 1D monatomic metal chains, which shows enhanced magnetism and band narrowing of Co 3-d band. One dimensional (1D) nanowires show enhanced magnetism as compared to their bulk (3 dimensional) state and quantized conductance and predicted to be technologically extremely useful for the future spintronics based devices. We have used density functional theory (DFT) and mean field (MF) results together to explain the magnetic phenomenon in 1D monatomic chain of 3d transition elements. The results shows that in ferromagnetic ground state band-width of both spins become different due to combined effect of band splitting and relative band narrowing/broadening. The relative band narrowing/broadening plays a crucial role and is a manifestation of correlated hopping interaction. We have done the study by making two groups as per their band filling. Sc, Ti, V and Cr have less than half filled band and we have found that the up spin band broadens and down spin band narrowed down. Mn, Fe, Co and Ni was treated in the category of half-filled and more than half filled band and found that the down spin band broadens and up spin band narrowed down. It was observed that, (in most of the cases) only one spin channel is present for conduction and there is relative bandwidth correction occurs within the DFT results. The attempt was made to find an answer using extended Hubbard model within MF approximation. In the absence of off-diagonal matrix elements (i.e., no bandwidth correction emerges), the system is driven by usual band splitting phenomenon. Hence a mapping has been done between DFT and MF results. It is found that correlation effects become more profound at low dimension, and one must consider the electron correlations by including the off-diagonal matrix elements of Coulomb interaction as it is evident from the present study, the correlated hopping plays an important role to understand the physics of low dimensional itinerant ferromagnets.

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