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Theoretical investigation of noncollinear magnetism for Mn_5 and Mn_6[1] TSUGUO MORISATO, SHIV KHANNA, Physics Department, Virginia Commonwealth University, Richmond, VA 23284-2000, U. S. A., YOSHIYUKI KAWAZOE, Institutes for Materials Research, Tohoku University, Sendai, 980-8577, Japan — The presence of odd-number rings in systems marked by nearest -neighbor antiferromagnetic (AFM) coupling can lead to situations where it is not possible to satisfy all interactions to find the ground state. This leads to so called "frustration." Since atomic clusters tend to take structures containing triangles or tetrahedra, this can cause magnetic frustration. It is therefore possible that some transition metals like chromium or manganese, whose crystals tend to be AFM, show noncollinear (NCL) magnetic configuration in small clusters. In the present study, we carry out first-principles calculations with NCL magnetism for Mn_5 and Mn_6 clusters. We adopt the projected augmented-wave method of the program called VASP (Vienna *ab initio* simulation package) for this calculation. From the results, we can see Mn_5 may take NCL magnetic configuration as one of the ground states isomers, while other isomers have collinear configurations. For the Mn_6, we found the NCL magnetic configuration is highly expected as the ground state.

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