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Enhanced magnetic moments of Sc, Ti and V doped Na_n(n =4, 5, 6) clusters[1] J. ULISES REVELES, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284, USA, KALPATARU PRADHAN, PRASENJIT SEN, Harish-Chandra Research Institute, Allahabad 211019, INDIA, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284, USA — Theoretical studies on the geometry, electronic structure and spin multiplicity of Sc, Ti and V doped Na_n (n = 4, 5, 6) clusters have been carried out within a gradient corrected density functional approach. Two complementary approaches including all-electron calculations on free clusters, and supercell calculations using planewave pseudopotential and projector augmented wave formalisms have been carried out. It is shown that spin magnetic moments of the transition metal atoms, the magnitude of host polarization, and the sign of the host polarization all change with the number of alkali atoms. In particular the transition metal atoms are shown to attain spin moments that are higher than their atomic values. The role of hybridization between the transition atom *d*-states and the alkali *sp*-states is highlighted to account for the evolutions in the spin moments and host polarization.

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