

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic structure of vitamin B₁₂ within the framework of the Haldane-Anderson impurity model ZAFER KANDEMIR, SELMA MAYDA, NEJAT BULUT, Izmir Inst of Tech — We study the electronic structure of vitamin B₁₂ (cyanocobalamine C₆₃H₈₈CoN₁₄O₁₄P) by using the framework of the multi-orbital single-impurity Haldane-Anderson model of a transition-metal impurity in a semiconductor host. Here, our purpose is to understand the many-body effects originating from the transition-metal impurity. In this approach, the cobalt *3d* orbitals are treated as the impurity states placed in a semiconductor host which consists of the rest of the molecule. The parameters of the resulting effective Haldane-Anderson model are obtained within the Hartree-Fock approximation for the electronic structure of the molecule. The quantum Monte Carlo technique is then used to calculate the one-electron and magnetic correlation functions of this effective Haldane-Anderson model for vitamin B₁₂. We find that new states form inside the semiconductor gap due to the on-site Coulomb interaction at the impurity *3d* orbitals and that these states become the highest occupied molecular orbitals. In addition, we present results on the charge distribution and spin correlations around the Co atom. We compare the results of this approach with those obtained by the density-functional theory calculations.

Nejat Bulut
Izmir Inst of Tech

Date submitted: 13 Nov 2014

Electronic form version 1.4