

Ground state of Ho atoms on Pt(111) metal surfaces: implications for magnetism.

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Rok wydania

2016

Czasopismo

Physical Review B

Numer woluminu

93

Strony

1-7

DOI

10.1103/PhysRevB.93.184415

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

We investigated the ground state of Ho atoms adsorbed on the Pt(111) surface, for which conflicting results exist. The density functional theory (DFT) calculations yielded the Ho ground state as $|J_z=\pm 8\rangle$. Interpretation of x-ray absorption spectroscopy and x-ray magnetic circular dichroism spectra and the magnetization curves indicated the ground state as $|J_z=\pm 6\rangle$. Superposition model is employed to predict the crystal-field (CF) parameters based on the structural data for the system Ho/Pt(111) obtained from the DFT modeling. Simultaneous diagonalization of the free-ion(HFI) and the trigonal CF Hamiltonian(HCF) within the whole configuration $4f^{10}$ of Ho^{3+} ion was performed. The role of the trigonal CF terms, neglected in the pure uniaxial CF model used previously for interpretation of experimental spectra, is found significant, whereas the sixth-rank CF terms may be neglected in agreement with the DFT predictions. The results provide substantial support for the experimental designation of the $|J_z=\pm 6\rangle$ ground state, albeit with subtle difference due to admixture of other $|J_z\rangle$ states, but run against the DFT-based designation of the $|J_z=\pm 8\rangle$ ground state. A subtle splitting of the ground energy level with the state (predominantly) $|J_z=\pm 6\rangle$ is predicted. This paper provides better insight into the single-ion magnetic behavior of the Ho/Pt(111) system by helping to resolve the controversy concerning the Ho ground state. Experimental techniques with greater resolution powers are suggested for direct confirmation of this splitting and C_{3v} symmetry experienced by the Ho atom.

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<http://dx.doi.org/10.1103/PhysRevB.93.184415>

Plik został wygenerowany dnia 2026-10-08 00:49:46

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