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Stability, electronic and magnetic properties of small M-doped Rhodium clusters

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Abstract

The geometries, relative stabilities, electronic and magnetic properties of small Rh_nM (M = Rh, Al, Co, V) ($n \leq 8$) clusters were investigated by employing the density functional theory (DFT). CALYPSO method (structure analysis by a particle swarm optimization algorithm) was used to search the structures. The doping of V atom in Rh clusters can enhance the stability of host clusters due to the strong Rh-V interaction. The magnetic moment of Rh clusters can be enhanced by doping Co atom because of the large local magnetic moment of Co atom and the ferromagnetic coupling of Co and Rh atoms. Magnetic moments of the studied clusters are dominantly contributed by d electrons of metal atoms.

Keywords: CALYPSO method, DFT, transition-metal clusters, magnetic properties.

1. Introduction

As compared to atomic and bulk counterparts, clusters are not only good catalysts but good magnetism materials [1]. Especially, transition-metal (TM) clusters always receive much attention and have been applied in many fields due to their special physical and chemical properties, which may be tuned by controlling their chemical composition and the size [2, 3]. Among the 3d, 4d, and 5d TM clusters, rhodium clusters have attracted extensive attention because of the wide range of applications in

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