量子物理学・ナノサイエンス第 210 回セミナー

Influence of nitrogen dopants on the magnetization of Co_3N clusters

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概　要

Using a real-space pseudopotential approach within the density-functional theory, which is implemented in the PARSEC code, we examine the structural stability and magnetic properties of Co_3N clusters with recently-discovered atomic structures [1]. We show that nitrogen dopants can have a notable influence on the magnetization of Co_3N clusters depending on the atomic structure of a cluster. We clarify that the changes in the magnetic moments due to nitrogen doping originate from the difference in an orbital hybridization between the Co 3*d* and N 2*p* states. We find that the total magnetic moment of a Co_3N cluster can be enhanced further by controlling the amount of nitrogen dopants.

[1] M. Sakurai, X. Zhao, C.-Z. Wang, K.-M. Ho, and J. R. Chelikowsky, to be submitted.

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