



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

講師 : 櫻井 誠大 氏

University of Texas, Austin

日程 : 12 月 26 日 (火) 11:00-

場所 : 本館 2 階 H284A 物理学系輪講室

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 $3d$ and N $2p$ 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.

連絡教員 物理学系 斎藤 晋 (内線 2070)
