量子物理学・ナノサイエンス第 33 回特別セミナー

Structural and magnetic properties of cobalt and nickel clusters: a real-space pseudopotential study

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概　要

We studied the structural stability and magnetic property of transition-metal clusters from first principles [1-2]. The use of our first-principles code, PARSEC, which employs a real-space formalism of pseudopotentials within the density-functional theory, enabled us to examine magnetic clusters of cobalt and nickel with a size range well beyond the previous work. The calculated total magnetic moments per atom agree well with experiment, wherein the moments decrease non-monotonically toward the bulk value as cluster grows in size. We analyzed the spatial distribution of the local magnetic moment, which explains the enhancement of the net magnetic moments in Co and Ni clusters. We also examined the effect of nitrogen substitution on the magnetic properties of Co clusters. A few atomic percent of N substitution can further enhance the total magnetic moment in comparison to that of pure Co cluster, where a N-substitution site plays a key role for the enhancement.

REFERENCES:
[1] J. Souto-Casares, M. Sakurai, and J. R. Chelikowsky, Structural and magnetic properties of large cobalt clusters, Phys. Rev. B **93** 174418 (2016).
[2] M. Sakurai, J. Souto-Casares, and J. R. Chelikowsky, Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials, Phys. Rev. B **94** 024437 (2016).

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