Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Effect of nitrogen substitution on the magnetic property of cobalt clusters[1] MASAHIRO SAKURAI, JAMES R. CHELIKOWSKY, University of Texas at Austin — We investigate the effect of nitrogen substitution on the magnetic property of cobalt clusters using a real-space formalism of pseudopotentials within the density-functional theory, i.e., the PARSEC code. We find that a few atomic percent of N substitution can enhance the net magnetic moment in comparison to that of pure Co cluster. An analysis of the spatial distribution of the local magnetic moment reveals the importance of a N-substitution site in Co cluster. By using the PARSEC code in a non-collinear magnetic mode, which enables us to explore various magnetic structures, the effect of N substitution on the magnetic anisotropy in Co cluster will also be discussed.

[1]This work is supported by grant from the National Science Foundation, DMREF-1435219 and by XSEDE.

James Chelikowsky
Univ of Texas, Austin

Date submitted: 09 Nov 2016 Electronic form version 1.4