Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic, magnetic and oxidation properties of Co and $Co_{1-x}Ni_x$ subnanoscopic cylinders EUGENIO VOGEL, Universidad de La Frontera, Chile, J. MARTIN MONTEJANO-CARRIZALES, FAUTINO AGUILERA-GRANJA, Universidad Autonoma San Luis Potosi, Mexico — One of the most convenient shapes among magnetic nanoparticles are cylinders (solid or hollow). They can be made out of different materials, they are easy to produce in different sizes, and they are relatively easy to handle. One of the present aims at present it to make these particles as small as possible. Which is the minimum stable cylindrical shape possible? Can they grow from a seed to make large particles? What are their physical properties at this scale where quantum mechanics operate? Some of these questions have been recently answered for the case of cylinders formed by Co atoms [F. Aguilera-Granja, J.M. Montejano-Carrizales, E.E. Vogel, Eur. Phys. J. D (2014) **68**:38]. In this presentation we want to get deeper into this problem in particular considering binary magnetic alloys like it is the case when Ni atoms substitute for Co in the original stable structures. We invoke program SIESTA to study different configurations. Among the results to be reported are the following: cylindrical clusters are stable to any length at this scale; there is an insulator-conductor transition at a certain length; magnetic moments are not uniformly distributed; Ni atoms tend to go to the periphery; Ni alloys tend to be more resistant to oxidation.

Eugenio Vogel
Universidad de La Frontera

Date submitted: 29 Sep 2014 Electronic form version 1.4