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Are catalytic properties preserved at the nanoscale?: The case of cobalt.[1] FERNANDO REBOREDO, GIULIA GALLI, Lawrence Livermore National Lab. — It is generally believed that the chemical activity of metal catalysts would be increased at the nanoscale because of the increment of surface to volume ratio. However, reducing the size of a metal particle to few hundred of atoms changes its electronic and chemical properties, with respect to the bulk. Therefore, whether small metal nanoparticles remain good catalyst or are better catalysts than bulk materials remains an open question. Bulk cobalt surfaces are known to catalyze important chemical reactions. In this talk we report ab-initio calculations of the chemisorption of CO on small Co clusters, in particular chemisorption energies a function of the size of the Co cluster and the surface coverage. Our results show a significant change in the total magnetic moment of the clusters as a function of CO coverage, suggesting that Co clusters may be used as gas sensors. We also discuss the changes in catalytic activity of the cluster as a function of size.

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