Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

A first-principles study of the electropotential dependent shape stability of metal nanoparticles NICEPHORE BONNET, MIT, ISMAILA DABO, CERMICS ENPC, NICOLA MARZARI, MIT — Understanding the catalytic activity of transition metal nanoparticles is a central issue in the development of novel fuel cell materials. Observed trends are often interpreted in terms of the size dependent shape of nanoparticles, in particular the relative density of low coordination sites. However, no consensus exists regarding the direction or even the existence of such an effect. In this context, ab-initio methods can be useful to extract relevant parameters. Here, we calculate surface energies under realistic electrochemical conditions and use the Wulff construction to infer stable nanoparticle contours. The electropotential is adjusted through its conjugate variable, the charge, and density countercharge periodic-image corrections are applied. The surrounding solvent is treated as a combination of a continuum dielectric and a classical ionic distribution at equilibrium.

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Date submitted: 25 Nov 2008 Electronic form version 1.4