Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Generation of amorphous porous PdH: an *ab initio* approach ISAIAS RODRIGUEZ[1], Instituto de Investigaciones en Materiales, UNAM, RENELA VALLADARES, Facultad de Ciencias, UNAM, ARIEL A. VALLADARES, Instituto de Investigaciones en Materiales, UNAM, ALEXANDER VALLADARES, Facultad de Ciencias, UNAM — The hydrogen bubble template (HBT) method has been employed to generate amorphous porous structures in platinum, nickel, copper and gold. We used our *ab initio* approach to generate amorphous porous $Pd_{50}H_{50}$; $Pd_{45}H_{55}$; $Pd_{40}H_{60}$, using an approach similar to the HBT method which keeps the interatomic distances the same as in the pure crystalline Pd, swapping palladium by hydrogen in a substitutional way, thus reducing the density and making the initial supercell metastable. We applied this HBT-like method to an initial 108-atom crystalline face-centered cubic palladium supercell, with an initial density of $12.02 g/cm^3$. After the substitution we got three supercells: a crystalline supercell: Pd54H54, with a density of $6.056 \frac{g}{cm^3}$; a supercell: Pd49H59, with a density of $5.506 \frac{g}{cm^3}$; and a supercell: Pd43H65, with a density of $4.846 \frac{g}{cm^3}$. After the hydrogen insertion an MD process at $1000 K$ was applied, and the resulting structures finally relaxed. Pores appeared along well-defined spatial directions. We characterized the structures by means of the pair distribution function (PDF) and the bond-angle distribution. Our results will be discussed in the light of possible structures of amorphous porous palladium hydride.

[1]Supported by CONACYT and DGAPA, UNAM.

Isaias Rodriguez
Instituto de Investigaciones en Materiales, UNAM

Date submitted: 14 Nov 2013 Electronic form version 1.4