Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

CO Adsorption on Pd(111) at 0.5ML: a First Principles Study[1]
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— While the adlayer structures formed by CO molecules on Pd(111) are well-understood both experimentally and theoretically, for low and high coverages, it is still a matter of discussion for medium coverage (0.5ML). At this medium coverage, it is well-known that the c(4 $\times$ 2) phase is formed but the adsorption sites of CO molecules have been reported differently by various studies: at the bridge sites, at the hollow sites, or at both bridge and hollow sites. Using density functional theory calculations we studied the overlayer structure of CO at 0.5ML on Pd(111) with all possible highly symmetric adsorption sites leading to c(4 $\times$ 2) structures. We will show that, on the same surface, CO molecules adsorb either only on bridge or hollow sites and that there is no overlayer structure in which CO binds at both bridge and hollow sites. By means of *ab initio* thermodynamics simulation, we will also report the conditions (temperature, pressure) in which each overlayer structure exists.

[1]Work support in part by NSF Grant CHE-1310327

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Date submitted: 14 Nov 2014 Electronic form version 1.4