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CO Adsorption on Pd(111) at 0.5ML: a First Principles Study¹ ZAHRA HOOSHMAND GHAREHBAGH, DUY LE, TALAT RAHMAN, University of Central Florida, ZAHRA HOOSHMAND GHAREHBAGH, DUY LE, TALAT RAHMAN TEAM — While the overlayer 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 (0.5 ML). At this coverage, it is well-known that the c(4 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 $c(4 \ 2)$ structures. We will show that CO molecules adsorb only on hollow sites and that there is no overlayer structure in which CO binds at both bridge and hollow sites or bridge sites only. By simulating Scanning Tunneling Microscopy (STM) images of obtained structures we could predict the one corresponding to the most frequently observed STM and correctly assign the experimental STM images to CO overlayer structures.

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