Abstract Submitted
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H Adsorption on RH (110) Surface SHAO-PING CHEN, Los Alamos National Laboratory — We have used the density functional theory to study the H adsorption phenomena on Rh (110) surface with H coverage from 0.33 to 2.00 mono-layers. We found H atom favors the three- fold coordinated site as observed experimentally. We confirmed the existence of 1x3-H, 1x2-H, 1x3-2H, 1x1-2H ordered structures. We also found that the proposed 1x2-2H structure for coverage of 1.0 is not the lowest energy configuration. We have proposed a new 1x2-2H structure which needs to be tested by future experiments.

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