

Abstract Submitted
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Adsorption and reaction of benzene and phenol with Pd nanoparticles supported on TiO₂(110)¹ J. ZHOU, S. V. KALININ, S. DAG, V. MEUNIER, S. H. OVERBURY, D. R. MULLINS, A. P. BADDORF, Oak Ridge National Laboratory — Adsorption and reaction of benzene and phenol molecules on a TiO₂(110)(1×1) surface and with titania-supported Pd particles were studied under ultrahigh vacuum conditions using scanning tunneling microscopy (STM) and temperature programmed desorption (TPD). At 300 K, benzene could not be imaged with STM due to its high mobility. At 20 K, images show benzene in ordered rows on top of substrate Ti. Adsorption of phenol differs due to the presence of the OH functional group. At 300 K, adsorption of phenoxy adjacent to surface defects is indicated in STM images. Low temperature studies indicate that phenol adsorbs on the titania surface with a different configuration than benzene, with tunneling spanning two Ti rows. No obvious modifications to benzene or phenol adsorption were observed adjacent to Pd particles by STM, however catalytic effects were explored by TPD. Our results are in excellent agreement with calculations obtained using first-principles density functional theory.

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