

Abstract Submitted
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A theoretical study of adsorption of NO on RuO₂(110) SAMPYO HONG, TALAT RAHMAN, Kansas State University — Experiments suggest that while RuO₂(110) is a highly reactive surface for CO oxidation, the same is not the case for NO adsorbed on this surface [1]. In order to understand the rationale for this difference, we have carried out *ab initio* electronic structure calculations to examine the idiosyncrasies in the adsorption, dissociation, and oxidation processes for CO and NO on RuO₂(110). Our calculated geometry and adsorption energies for NO adsorption are in good agreement with experiments available. Our results confirm that while CO can easily oxidize on this surface [2], NO does not bind easily to the bridging O atoms to produce NO₂. Detailed analysis of the surface electronic structure, including the charge transfer, charge density distribution and local electronic density of states together with its hybridization is presented to compare and contrast the energetics and dynamics of CO and NO on RuO₂(110). [1] Y. Wang, K. Jacobi, and G. Ertl, J. Phys. Chem. B **107**, 13918 (2003). [2] Z. Liu, P. Hu, A. Alavi, J. Chem. Phys. **114**, 5956 (2001).

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