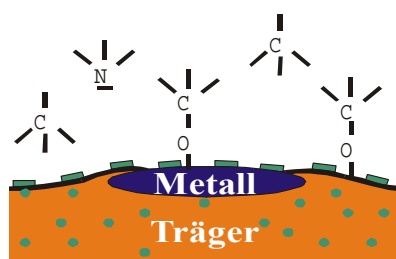


Ruhr-Universität Bochum



SFB 558

„Metall-Substrat-Wechselwirkungen in der heterogenen Katalyse“

Einladung
zum Vortrag von

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(Gast von Prof. Wöll)**

“A Novel Consequence of the Pauli Exclusion Principle: Adsorbate Induced Changes in the Interface Dipole”

Abstract: It is common to relate changes in the interface dipole, induced by the presence of adsorbates on a surface, and the consequent changes in the work function to the charge residing on the adsorbate. In particular, large work function changes can result from charge transfer between the substrate and the adsorbate. However, it has been recognized for some time,^{1,2} that factors other than charge transfer can contribute to changes in the interface dipole. An important contribution may arise from the polarization of the surface charge density induced by the presence of the adsorbate; this will be especially important when the adsorbate is charged. Recently, it has been shown that the quantum mechanical requirement that electronic wavefunctions are anti-symmetric with respect to exchange of electron coordinates can lead to major changes in the interface dipole.^{3,4} This requirement, also described as the Pauli exclusion principle, involves only physical changes in the charge distributions, as contrasted to changes involving chemical bonding. It leads to an exchange-like “correction” to the dipole moment. Initially, this consequence of the Pauli exclusion principle was investigated for weakly bound adsorbates like Xe³ and alkanes⁴ where it is a dominant origin of the changes in the interface dipole. Here, we extend the prior analyses to cases where there is a strong covalent bond including CO adsorbed on metal surfaces where the overlap of the 5σ lone pair with the surface charge density makes the Pauli exclusion effect on the dipole moment significant. The dependence of the various contributions to the interface dipole on the distance between the adsorbates and the surface are examined. The dependence of these contributions on the bond distance, especially that of the Pauli exclusion contribution, raises the intriguing possibility that interface work function changes could be tuned by choosing systems with suitable bond distances. In particular, using the adsorbate-substrate distance as a criterion for the magnitude of work functions changes may be most useful for weakly bound adsorbates.

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