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Titel des Beitrags:
Charging Effects on Bonding and Catalyzed Oxidation of CO on Au8 Clusters on MgO

Abstract:
Gold octamers (Au8) bound to oxygen-vacancy F-center defects on Mg(001) are the smallest clusters to catalyze the low-temp. oxidn. of CO to CO2, whereas clusters deposited on close-to-perfect magnesia surfaces remain chem. inert. Charging of the supported clusters plays a key role in promoting their chem. activity. IR measurements of the stretch vibration of CO adsorbed on mass-selected gold octamers soft-landed on MgO(001) with coadsorbed O2 show a red shift on an F-center-rich surface with respect to the perfect surface. The expts. agree with quantum ab initio calcns. that predict that a red shift of the C-O vibration should arise via electron back-donation to the CO antibonding orbital. [on SciFinder(R)]

Stichworte:
Oxidation (catalytic charging effects on bonding and catalyzed oxidn. of CO on Au8 clusters on MgO) Ab initio methods Adsorbed substances Binding energy Bond Density of states Electric charge F-centers IR spectra Molecular orbital Oxidation catalysts (charging effects on bonding and catalyzed oxidn. of CO on Au8 clusters on MgO) bonding catalyzed oxidn carbon monoxide gold cluster magnesia charging effect catalyzed oxidn carbon monoxide gold cluster magnesia ir spectrum catalyzed oxidn carbon monoxide gold cluster magnesia

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Reaction Mechanisms School of Physics, Georgia Institute of Technology, Atlanta, GA, USA. Journal 0036-8075 1309-48-4 (Magnesia); 145536-84-1 Role: CAT (Catalyst use), PRP (Properties), USES (Uses) (charging effects on bonding and catalyzed oxidn. of CO on Au8 clusters on MgO); 630-08-0 (Carbon monoxide); 7782-44-7 (Oxygen) Role: CPS (Chemical process), PEP (Physical, engineering or chemical process), PRP (Properties), RCT (Reactant), PROC (Process), RACT (Reactant or reagent) (charging effects on bonding and catalyzed oxidn. of CO on Au8 clusters on MgO)

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