Fakultät für Chemie

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Titel des Beitrags:
Conversion of NO to N2O on MgO Thin Films

Abstract:
No adsorption on ultra-thin MgO films grown on a Mo(100) substrate result in formation of N2O at low temp. (120 K). Also, small amts. of N2O are produced at 280 K. Isotope exchange expts. showed the reaction does not involve lattice O. Ab-initio DFT/B3LYP cluster model calcns. were performed to understand the reaction mechanism, considering various defect sites on the MgO surface. The reaction occurs preferentially at neutral O vacancies (F centers) via adsorption of a first NO mol. followed by the addn. of a second NO; from the adsorbed dimer, N2O2, N2O forms with an activation barrier of ∼0.1 eV, leaving a regular site instead of the original F center. This result is consistent with expn. observations that subsequent exposure of the surface to NO results in reduced N2O prodn. [on SciFinder(R)]

Stichworte:
Reduction catalysts (magnesium oxide thin films reaction temp. and oxygen vacancy effect on exhaust gas nitric oxide conversion to nitrous oxide following adsorption on ultra-thin magnesium oxide films grown on molybdenum substrate) Adsorption Exhaust gases (reaction temp. and oxygen vacancy effect on exhaust gas nitric oxide conversion to nitrous oxide following adsorption on ultra-thin magnesium oxide films grown on molybdenum substrate) nitric oxide conversion nitrous oxide magnesium oxide thin film exhaust gas nitric oxide conversion redn catalyst molybdenum supported magnesium oxide thin film catalyst