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Titel des Beitrags:
Nano-assembled Pd catalysts on MgO thin films

Abstract:
Cluster-assembled materials open fascinating new routes for tuning phys. and chem. properties by changing cluster size and often behave completely differently than their bulk analogs. By depositing gas phase Pd clusters on MgO thin films, model catalysts are fabricated which exhibit remarkable catalytic activity. In contrast to the high selectivity of Pd (111) surfaces for the cyclotrimerization of acetylene to benzene, small supported Pd clusters reveal a strongly size-dependent selectivity and catalyze the formation of benzene as well as of other hydrocarbons. The understanding at the atomistic level of the obsd. processes has been obtained by means of first-principles quantum-mech. simulations. The theor. studies have shown the importance of the surface defects of the oxide substrate in stabilizing the supported clusters but also in promoting their catalytic activity. For instance, Pd atoms bound at the regular sites of the MgO (100) terraces do not promote the acetylene to benzene conversion while they become active catalysts when bound at oxygen vacancies (F centers). [on SciFinder(R)]

Stichworte:
Cyclotrimerization catalysts (for acetylene nano-assembled Pd catalysts on MgO thin films) Clusters Role: CAT (Catalyst use), PRP (Properties), USES (Uses) (metal nano-assembled Pd catalysts on MgO thin films) Catalyst supports Catalysts Simulation and Modeling