Nano-assembled Pd catalysts on MgO thin films

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 Pdn 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)]

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
Surface defects (nano-assembled Pd catalysts on MgO thin films) nano assembled palladium catalyst magnesia thin film

Kongressstitel: CAN 136:43437 67-1 Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms Institut de Physique de la Matiere Condensee, Universite de Lausanne, Lausanne, Switz. Journal 0040-6090 74-86-2 (Acetylene) Role: RCT (Reactant), RACT (Reactant or reagent) (cyclotrimmerization of; nano-assembled Pd catalysts on MgO thin films); 1309-48-4 (Magnesia); 7440-05-3D (Palladium) Role: CAT (Catalyst use), PRP (Properties), USES (Uses) (nano-assembled Pd catalysts on MgO thin films)

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