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Articles

Dmitry Yu. Murzin

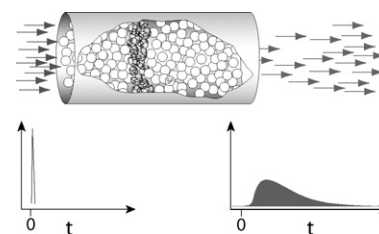
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The man behind the name: Professor Mikhail Temkin

John T. Gleaves, Gregory Yablonsky, Xiaolin Zheng, Rebecca Fushimi, Patrick L. Mills

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Temporal analysis of products (TAP)—Recent advances in technology for kinetic analysis of multi-component catalysts

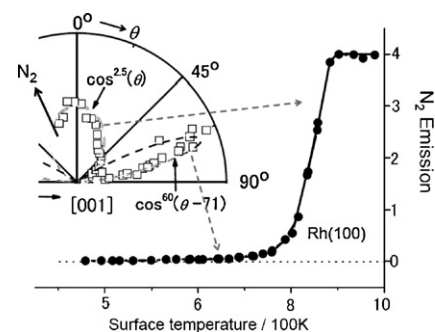


Tatsuo Matsushima, Kosuke Shobatake

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Surface reaction dynamics and energy partitioning

Product N_2 intensity in NO reduction on Rh(1 0 0) versus surface temperature and its angular distribution at 664 K. The inclined emission comes from the decomposition of intermediate N_2O . Above about 700 K, the normally directed component due to combinative desorption of nitrogen adatoms predominates.

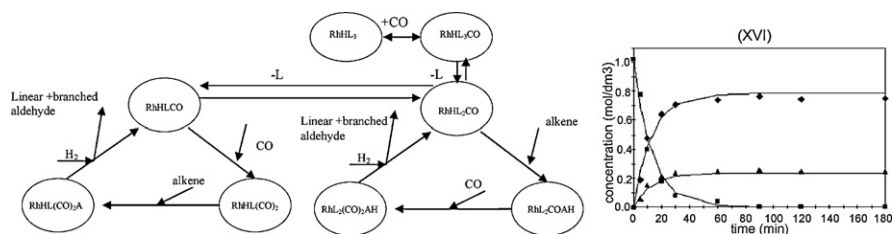


Dmitry Yu. Murzin, Andreas Bernas, Tapio Salmi

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Kinetic modelling of regioselectivity in alkenes hydroformylation over rhodium

Propene hydroformylation was performed with rhodium triphenylphosphine catalyst varying hydrogen and CO partial pressure in the range of 8–15 bar. The regioselectivity was independent on the concentration of reactants, displaying dependence on the ligand concentration. A kinetic model was proposed based on the mechanism of alkene hydroformylation and compared with experimental observations. Numerical data fitting was performed showing good correspondence of reaction rates and isoselectivity with experimental data.

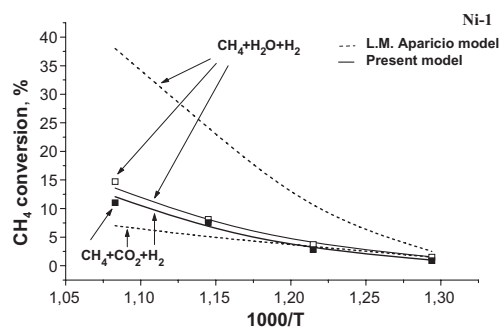


A.K. Avetisov, J.R. Rostrup-Nielsen, V.L. Kuchaev, J.-H. Bak Hansen, A.G. Zyskin, E.N. Shapatina

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Steady-state kinetics and mechanism of methane reforming with steam and carbon dioxide over Ni catalyst

Based on new own and known published experimental data a microkinetic model of steam and dry methane reforming on Ni-catalyst is proposed and proved. The model eliminates drawbacks of the known previous models. The kinetic equations are derived.

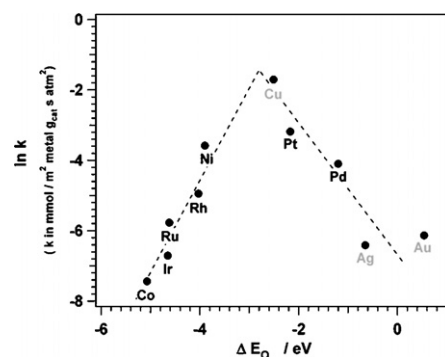


A. Boisen, T.V.W. Janssens, N. Schumacher, I. Chorkendorff, S. Dahl

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Support effects and catalytic trends for water gas shift activity of transition metals

Catalytic trends for water gas shift activity of transition metals were investigated for two supports. Trends are clearly different for the two supports.

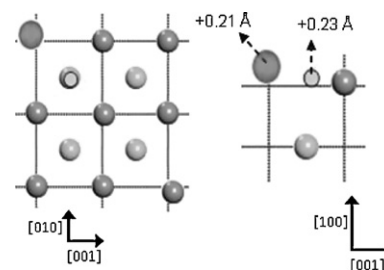


Hernán Milberg, Alfredo Juan, Norma Amadeo, Beatriz Irigoyen

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The influence of Mg on the C adsorption on Ni(1 0 0): A DFT study

We performed density functional theory (DFT) calculations to study the influence on Mg on carbon adsorption on the Ni(1 0 0) surface. Carbon adsorption on the bare Ni(1 0 0) surface is more favorable than deposition on this surface doped with magnesium. Our results also show that Mg could improve the interaction of surface adsorbed carbon with gas phase oxygen.

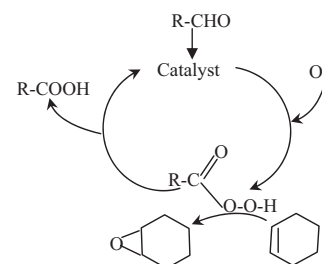


E. Angelescu, R. Ionescu, O.D. Pavel, R. Zăvoianu, R. Bîrjega, C.R. Luculescu, M. Florea, R. Olar

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Epoxidation of cyclohexene with O_2 and isobutyraldehyde catalysed by cobalt modified hydrotalcites

The paper presents a comparison between the catalytic performances of cobalt modified hydrotalcites obtained from different cobalt precursors in the epoxidation of cyclohexene using molecular oxygen, isobutyraldehyde as reductant, at 25 °C and 1 atmosphere pressure of oxygen in acetonitrile as solvent.

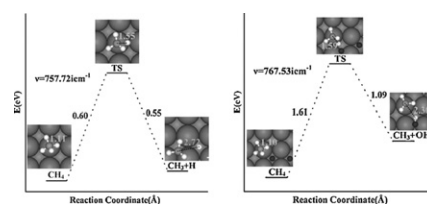


Bin Xing, Xian-Yong Pang, Gui-Chang Wang, Zhen-Feng Shang

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Investigation the active site of methane dissociation on Ni-based catalysts: A first-principles analysis

DFT results showed that the activation energy of methane decomposition on oxygen-pre-covered Ni(1 0 0) is larger than that of clean Ni(1 0 0), suggesting the activate site is the metallic Ni site. It was found that the presence of oxygen atom decreases the interaction of CH_3 and H with substrate in TS, which inhibits the dissociation of methane on Ni surface.

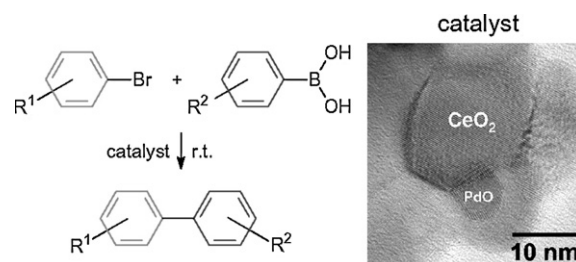


Francesco Amoroso, Sara Colussi, Alessandro Del Zotto, Jordi Llorca, Alessandro Trovarelli

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An efficient and reusable catalyst based on Pd/CeO₂ for the room temperature aerobic Suzuki–Miyaura reaction in water/ethanol

At room temperature in air Pd/CeO₂ efficiently catalyzes the Suzuki–Miyaura reaction in ethanol/water. This catalyst system promotes the quantitative conversion of several substrates and can be recycled at least ten times without loss of activity.

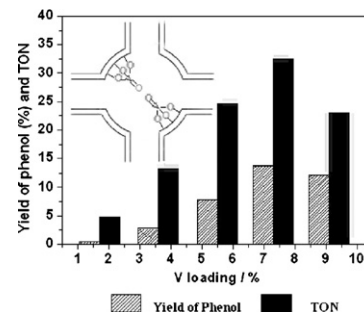


Yujun Zhu, Yongli Dong, Lina Zhao, Fulong Yuan

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Preparation and characterization of Mesoporous VO_x/SBA-16 and their application for the direct catalytic hydroxylation of benzene to phenol

VO_x/SBA-16 catalyst with 7.3 wt% V loading showed excellent activity for the hydroxylation of benzene, which was attributed to the formation of highly dispersed VO₄ species and nanostructured V₂O₅ crystallite. The highest phenol yield and turnover number were 13.8% and 32.4 with a selectivity of 97.5%, respectively.

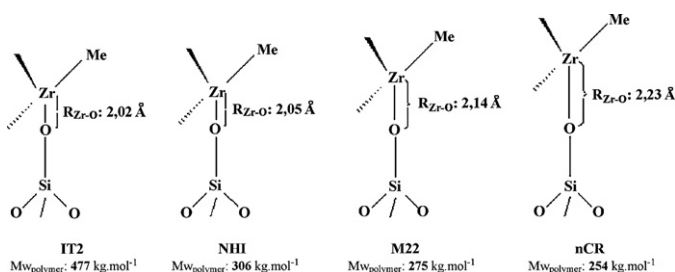


Fernando Silveira, Maria do Carmo Martins Alves, Fernanda C. Stedile, Sibebe B. Pergher, João Henrique Zimnoch dos Santos

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Microporous and mesoporous supports and their effect on the performance of supported metallocene catalysts

A series of hybrid-supported catalysts was prepared by sequentially grafting Cp_2ZrCl_2 and $(nBuCp)_2ZrCl_2$ (1:3 ratio) onto different mesoporous materials. The production of polyethylenes with higher molecular weight was associated to the reduction in the interatomic Zr–O distance of the supported catalysts, which was shown to be dependent on the nature of the support.

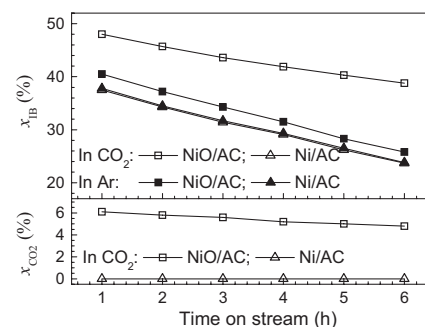


Jianfei Ding, Zhangfeng Qin, Xuekuan Li, Guofu Wang, Jianguo Wang

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Catalytic dehydrogenation of isobutane in the presence of carbon dioxide over nickel supported on active carbon

Dehydrogenation of isobutane to isobutene was carried out in CO_2 over NiO/AC. NiO and Ni species present in the catalyst are relevant to its calcination temperature. NiO and Ni species are different in the catalytic behaviors; Ni is only effective for direct dehydrogenation, while NiO is also highly active for the coupled dehydrogenation with CO_2 .

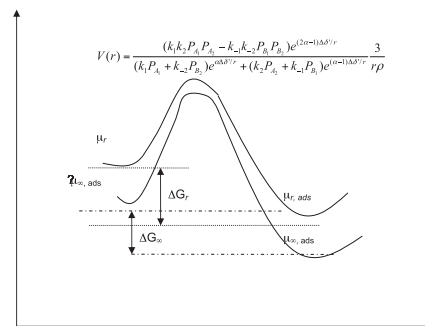


Dmitry Yu. Murzin

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Size-dependent heterogeneous catalytic kinetics

A quantitative thermodynamic approach is considered with the aim to describe the size-dependent Langmuir–Hinshelwood mechanism and the two-step catalytic cycle. The general treatment takes into account surface energy excess due to an intrinsic increase in chemical potential with size decrease as well as the changes in chemical potential upon adsorption.



V.V. Saraev, P.B. Kraikovskii, D.A. Matveev, V.V. Bocharova, S.K. Petrovskii, S.N. Zelinskii, A.I. Vilms, Hans-Friedrich Klein

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Cycloisomerization and [2 + 2]cycloaddition of 1,5-cyclooctadiene catalyzed with the $Ni(COD)_2/BF_3 \cdot OEt_2$ system

A fundamental possibility is shown for the formation of the cationic nickel(I) complexes stabilized in solution by olefin ligands.

