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Articles

Adelina M. Voutchkova, Robert H. Crabtree

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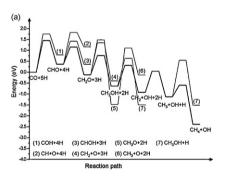
Iridium-catalyzed benzylic C–H activation and functionalization of alkyl arenes

Xue-Rong Shi, Haijun Jiao, Klaus Hermann, Jianguo Wang

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CO hydrogenation reaction on sulfided molybdenum catalysts

CO hydrogenation mechanisms at sulfur covered $MoS_2(1\ 0-1\ 0)$ surfaces are investigated systematically using periodic density functional theory. Calculated energies of possible reaction steps and barriers are used to identify optimized reaction paths.

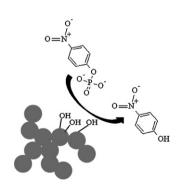


Joelle Akl, Tarek Ghaddar, Aline Ghanem, Houssam El-Rassy

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Cobalt ferrite aerogels by epoxide sol–gel addition: Efficient catalysts for the hydrolysis of 4-nitrophenyl phosphate

Porous cobalt ferrite aerogel catalysts were prepared by epoxide sol–gel process and characterized by FTIR, $\rm N_2$ adsorption and XRD. These solids were used in the hydrolysis of 4-nitrophenyl phosphate.



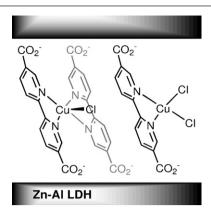
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Bernardo Monteiro, Sandra Gago, Salete S. Balula, Anabela A. Valente, Isabel S. Gonçalves, Martyn Pillinger

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Liquid-phase oxidation catalysed by copper(II) immobilised in a pillared layered double hydroxide

An LDH-supported copper(II) catalyst and the complex $[Cu(bipy)Cl_2]$ were tested in the oxidation of styrene, ethylbenzene and cyclohexane, using aqueous H_2O_2 or tert-butyl hydroperoxide as oxidant.

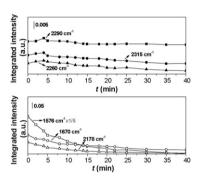


Xiaomei Chen, Xuefeng Yang, Aimin Zhu, C.T. Au, Chuan Shi

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In situ DRIFTS study during C_2H_4 -SCR of NO over Co-ZSM-5

The selective catalytic reduction of NO by ethylene has been investigated over Co-ZSM-5 by using *in situ* DRIFTS. Formate species are reactive towards nitrates to form formyl nitro compound, a precursor for formation of cyanide and isocyanate species. Kinetics analysis suggests that the cyanide and isocyanate at different sites vary in reactivity towards nitrates.



Wenshan Ren, Xiangkai Fu

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Chiral Mn (III) salen complexes covalently bonded on zirconium oligostyrenylphosphonate-phosphates as catalysts for enantioselective epoxidation of nonfunctionalized alkenes The chiral Mn (III) salen complex was supported on ZSPP by a covalent grafting method. These heterogeneous catalysts show comparable or even higher enantioselectivities than homogeneous chiral Mn (III) salen. The *x* values of ZSPP play an important role in ee values and yields of epoxidations. The heterogeneous catalysts are relatively stable and can be recycled nine times.

Tomonori Misaki, Hisafumi Otsuka, Takayuki Uchida, Takeshi Kubota, Yasuaki Okamoto, Takashi Sugimura

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Substrate adsorption on the cinchonidine-modified Pd/C during the enantio-differentiating hydrogenation as a vital stereocontrol factor

Cinchonidine-modified Pd/C effective for the enantioselective hydrogenation of phenylcinnamic acid was not effective for 4-Py and 3-Py under the standard conditions, but the ee with 4-Py improved at the low substrate/cinchonidine ratio.

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Clara Pereira, Krzysztof Biernacki, Susana L.H. Rebelo, Alexandre L. Magalhães, Ana Paula Carvalho, João Pires, Cristina Freire

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Designing heterogeneous oxovanadium and copper acetylacetonate catalysts: Effect of covalent immobilisation in epoxidation and aziridination reactions

VO(IV) and Cu(II) acetylacetonate complexes were immobilised onto organo-functionalised PCH and SBA-15. The catalytic activities of the novel heterogeneous catalysts were studied in the geraniol epoxidation and styrene aziridination, respectively. The supports effect on the immobilisation efficiencies and location of the complexes, and the influence of covalent grafting on the catalysts performance and stability were accessed and discussed.

K.T. Venkateswara Rao, P.S. Sai Prasad, N. Lingaiah

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Iron exchanged molybdophosphoric acid as an efficient heterogeneous catalyst for the synthesis of quinoxalines

A highly effective heterogeneous iron exchanged molybdophosphoric acid catalyst is reported for the one pot tandem oxidative cyclization of α -hydroxy ketones with 1,2-diamines under aerobic conditions. The plausible reaction mechanism is proposed based on reducible nature of Mo and Fe of the catalyst.

$$\begin{array}{c} R \longrightarrow OH \\ R \longrightarrow O \end{array} + \begin{array}{c} H_2N \longrightarrow \\ H_2N \longrightarrow \end{array} \begin{array}{c} FeMPA \longrightarrow \\ CH_3CN, O_2 \longrightarrow \\ reflex \longrightarrow \end{array} \begin{array}{c} R \longrightarrow N \longrightarrow \\ N \longrightarrow OH \end{array}$$

Nandi Malumbazo, Selwyn F. Mapolie

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Silica immobilized salicylaldimine Cu(II) and Co(II) complexes as catalysts in cyclohexene oxidation: A comparative study of support effects

Salicylaldimine complexes of Cu(II) and Co(II) immobilized on mesoporous silica were found to be active catalysts in the liquid phase oxidation of cyclohexene. All catalysts show high selectivity to allylic oxidation products with 2-cyclohexen-1-ol and 2-cyclohexen-1-one being produced in large amounts.

Maria A. Peralta, Tawan Sooknoi, Tanate Danuthai, Daniel E. Resasco

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Deoxygenation of benzaldehyde over CsNaX zeolites

The deoxygenation of benzaldehyde to benzene and toluene was investigated on basic zeolites. The CsNaX, containing Cs in excess, displays high activity for direct decarbonylation of benzaldehyde. In parallel, condensation of surface products occurs. Gas-phase $\rm\,H_2$ reduces catalyst deactivation by decreasing the amount of condensation products that accumulate on the surface.

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Ahlam Sibaouih, Paul Ryan, Kirill V. Axenov, Markku R. Sundberg, Markku Leskelä, Timo Repo

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Efficient coupling of CO₂ and epoxides with bis(phenoxyiminato) cobalt(III)/Lewis base catalysts

A series of unbridged bis(phenoxyiminato) cobalt(III)complexes were synthesized and studied as catalysts for the coupling of CO_2 and epoxide. Dimethylamino pyridine (DMAP) and tetrabutyl ammonium bromide (Bu₄NBr), were used as co-catalysts in the reaction. Both $\mathrm{Co}(\mathrm{III})/\mathrm{DMAP}$ and $\mathrm{Co}(\mathrm{III})/\mathrm{Bu}_4\mathrm{NBr}$ systems showed high catalytic activity and selectivity in the coupling of n-hexyl oxide and CO_2 , resulting in n-hexyl carbonate. Several mono- and di-substituted terminal epoxides were also tested. The reaction mechanism of the $\mathrm{Co}(\mathrm{III})/\mathrm{DMAP}$ system was investigated in detail using ESI-MS revealing that in addition to the main product, cyclic carbonate, traces of oligomers are formed.

E.A. Ivanov, G.Ya. Popova, Yu.A. Chesalov, T.V. Andrushkevich

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In situ FTIR study of the kinetics of formic acid decomposition on V–Ti oxide catalyst under stationary and non-stationary conditions. Determination of kinetic constants

Decomposition of formic acid over V–Ti oxide catalyst under stationary and non-stationary conditions was studied by *in situ* IR spectroscopy at temperature range 50-150 °C. The kinetic scheme was shown to include the steps of reverse adsorption of formic acid (A) and formate ([Z-A]) decomposition to CO.

The rate constants and activation energies were estimated according to the proposed kinetic model. The kinetic model satisfactorily describes the experimental data under stationary and non-stationary conditions.

$$A + [Z] \leftrightarrow [Z-A]$$

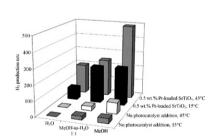
 $[Z-A] \rightarrow [Z] + CO + H_2O$

Tarawipa Puangpetch, Thammanoon Sreethawong, Susumu Yoshikawa, Sumaeth Chavadej

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Hydrogen production from photocatalytic water splitting over mesoporous-assembled SrTiO₃ nanocrystal-based photocatalysts

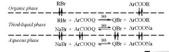
The main objective of this work is to present the application of a newly developed mesoporous-assembled ${\rm SrTiO}_3$ nanocrystal photocatalysts, synthesized by a ${\rm sol-gel}$ process with the aid of a structure-directing surfactant, for ${\rm H}_2$ production from water splitting reaction. The effects of hole scavenger type, hole scavenger concentration, and Pt co-catalyst loading were systematically studied. The reaction kinetics was investigated and analyzed. The reusability of the photocatalyst was also studied.



Hung-Ming Yang, Chien-Hsing Chen

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Catalytic esterification of sodium salicylate in thirdliquid phase under ultrasound-assisted tri-liquid phase-transfer catalysis Under 28 kHz/300 W of ultrasound-assisted third-liquid phase-transfer catalyzed esterification, the product yield in the organic phase was 97.4% after 100 min of reaction at 70 °C in a batch reactor.



Aqueous reactant: sodium salicylate (ArCOONa)
Organic reactant: n-butyl bromide (RBr)
Phase-transfer catalyst: tetra-n-butylphosphonium bromide (QI
Product: n-butyl salicylate (ArCOOR)

