Twelfth International Symposium on Heterogeneous Catalysis

Catalysis: a motor of economy

26–29 August 2018

Park Hotel Moskva, Sofia, Bulgaria

Programme

Programme
(as of 15th August 2018)

Sunday, 26th August 2018

10.00–19.00	**Registration and information**	
Europe Hall		
17:30–17:45	**Opening ceremony**	
17:45–18:30	**IL1-Invited lecture**: Revisiting ceria-NO_x interaction: FTIR studies	K. Hadjiivanov*, M. Y. Mihaylov, E. Z. Ivanova, H. A. Aleksandrov, P. St. Petkov, G. N. Vayssilov
18:30–19:15	**IL2-Invited lecture**: Direct desulphurisation for HDS of diesel fuel catalysed by MoS_2 dispersed over ordered mesoporous titania	J.-L. Blin*, S. Brunnet, B. Lebeau, I. Naboulsi, L. Michelin, M. Bonne
19.30	**Welcome reception at Forest restaurant**	

Monday, 27th August 2018

08:30–17:30	**Registration and information**	
Europe Hall		
09:00–09:45	**IL3-Invited lecture**: Structure-surface acidity relations on catalytic materials belonging to the SiO_2-Al_2O_3 system	G. Busca
09:45–10:30	**IL4-Invited lecture**: Recent approaches towards enhanced charge separation and visible light utilization in TiO_2 photocatalysis	A. Pintar
10:30–11:00	**Coffee break**	
11:00–11:45	**IL5-Invited lecture**: Ammonia synthesis with metal nitrides	J. S. J. Hargreaves
Oral contributions		
11:45–12:05	**O1**: Characterisation and activity studies on Ni-based pyrochlore catalysts for dry reforming of methane	S. Bhattar, A. Krishnakumar, S. Kanitkar, A. Abedin, D. Shekhawat, D. J. Haynes, J. J. Spivey*
12:05–12:25	**O2**: FTIR spectroscopy for the studies of catalysts and catalytic reaction mechanisms	A. Tsyganenko
12:30–13:30	**Lunch at Moskva restaurant**	

13:30–13:50	**O3**: Structural and acidic nature of phosphotungstic acid at the surface and in the bulk of silica: towards a heterogeneous catalyst for quinolones synthesis	P. Kasinathan*, E. M. Gaigneaux
13:50–14:10	**O4**: Stability of fly ash based Beta zeolite in hot liquid phase	A. E. Ameh*, C. P. Eze, E. Antunes, L. F. Petrik
14:10–14:30	**O5**: Investigation of the properties of Li^{+}, Co^{2+}, Mg^{2+}, Al^{3+} containing LDH prepared by mechanochemical route and used as support precursors for platinum containing catalysts	L. N. Stepanova*, O. B. Belskaya, A. V. Vasilevich, N. N. Leont'eva, O. N. Baklanova, V. A. Likholobov
14:30–14:50	**O6**: Facile and green route for the synthesis of SFE borosilicate zeolite and its heteroatom-substituted analogue with promising catalytic performance	Y. Luo, Z. Wang*, S. Jin, B. Zhang, H. Sun, W. Yang
14:50–15:10	**O7**: CO_2 hydrogenation over ceria-supported Pd-Zn based catalyst	S. F. Zaman*, A. S. Malik, A. A. Alzahrani, M. A. Daous
15:10–15:30	**O8**: Elimination reactions: dehydration of alkyl cyclohexanols with hydronium ions	P. H. Hintermeier, L. Milakovic, S. Eckstein, E. Baráth*, J. A. Lercher

Conference 3 Hall

Oral contributions

11:45–12:05	**O9**: Spatiotemporal operando DRIFTS study on NSR catalysts: comparative study on support materials	H. P. Nguyen*, J. Ampurdanés, A. Bansode, A. Urakawa
12:05–12:25	**O10**: Shell-isolated nanoparticle-enhanced Raman substrates for heterogeneous catalysis	T. Hartman*, B. M. Weckhuysen
12:30–13:30	**Lunch at Moskva restaurant**	
13:30–13:50	**O11**: Photocatalytic degradation of dyes using mesoporous TiO_2-based materials	F. Jonas*, I. Naboulsi, B. Lebeau, P. Gaudin, L. Michelin, M. Bonne, J. L. Blin
13:50–14:10	**O12**: Synthesis, characterisation and photocatalytic properties of WO_3/hexagonal platelet graphite nanocomposites	A. Y. S. Malkhasian*, K. Narasimharao
14:10–14:30	**O13**: Ferrites modified with Ag nanoparticles for photocatalytic degradation of Malachite Green in aqueous solutions	M. Tsvetkov*, J. Zaharieva, M. Milanova

14:30–14:50	**O14**: TiO_2-graphene nanocomposites: preparation, characterisation, and charge carrier transfer	E. Kusiak-Nejman*, D. Moszyński, A. Wanag, A. W. Morawski
14:50–15:10	**O15**: Bismuth silicate composite materials prepared *via* mechanochemical activation for photocatalytic applications	Yu. Belik, A. Vodyankin*, T. Kharlamova, O. Vodyankina
15:10–15:30	**O16**: Reduced graphene oxide supported monodisperse Ni-Pd core-shell nanoparticles as a highly efficient and reusable heterogeneous catalyst for the Suzuki-Miyaura coupling and C-H bond arylation reactions	Ö. Metin*, H. Kilic, M. Turgut, M. S. Yilmaz

15:30–16:00 **Coffee break**

Europe Hall

16:00–17:30 **Poster session**

P1: Understanding the effect of preparation method and Y-doped ceria loading on the water-gas shift activity of alumina-supported gold catalysts	T. Tabakova*, I. Ivanov, R. Zanella, P. Petrova, J. W. Sobczak, W. Lisowski, Z. Kaszkur, G. Munteanu, L. Ilieva
P2: Characterisation and catalytic activity in CO oxidation of biogenic lepidocrocite layered on anodic alumina	M. Shopska*, D. Paneva, H. Kolev, G. Kadinov, J. Briančin, M. Fabián, D. Kovacheva, Z. Cherkezova-Zheleva, I. Mitov
P3: CO and VOCs oxidation over Pt-based catalysts supported on Ti- and Ce-modified SBA-15 mesoporous silica	S. Todorova*, M. Shopska, M. Ciobanu, G. Petcu, F. Papa, S. Somacescu, D. Culita, S. Preda, V. Parvulescu
P4: Pd-Co/γ-Al_2O_3 catalysts supported on anodised alumina for complete oxidation of methane	S. Todorova*, B. Tzaneva, E. Uzunova, H. Kolev, G. Ivanov, A. Naydenov
P5: Electrocatalytic activity of electroless Ni-P alloy coating for hydrogen evolution reaction in acidic medium	V. Chakarova*, M. Monev
P6: Synthesis and properties of binary oxide V_2O_3+TiO_2 photocatalytic materials for waste water and air decontamination	A. Eliyas*, L. Dimitrov, V. Iliev, N. Kostova, E. Stoyanova
P7: Photocatalytic properties of $CaTiO_3$ in oxidative degradation of organic contaminants depending on the mechanochemical activation time	A. Eliyas*, I. Stambolova, V. Blaskov, K. Zaharieva, K. Milenova, D. Stoyanova, I. Avramova, L. Dimitrov

P8: Phthalocyanine-modified Au/TiO_2/reduced graphene oxide: catalyst for photooxidation of oxalic acid under irradiation with visible light	V. Iliev*, A. Eliyas, D. Tomova
P9: Synthesis-gas production by reforming of methane over Pt-Ru- and Ni-Cu-based nanosized catalysts	S. A. Tungatarova*, G. Xanthopoulou, T. S. Baizhumanova, Z. T. Zheksenbaeva, M. Zhumabek, K. Kassymkan, R. Sarsenova, G. Kaumenova, Y. Aubakirov, B. Massalimova, K. Shorayeva
P10: Flameless catalytic combustion of the methane of natural gas	Z. T. Zheksenbaeva, S. A. Tungatarova*, T. S. Baizhumanova, R. O. Sarsenova
P11: Impact of catalyst composition and reduction pretreatment on the activity in CO_2 removal by methanation reaction	M. Gabrovska*, R. Edreva-Kardjieva, D. Nikolova, P. Tzvetkov, M. Shopska, L. Biljarska
P12: Simple synthesis of raspberry ketone and the analogues by heterogeneous catalysed hydrogen-borrowing C-C bond formation	Y. Hori*, Y. Akabayashi, T. Myoda, K. Toeda
P13: Structure-oxidation activity relationship of monometallic and bimetallic Pd-Au catalysts for complete benzene oxidation	L. Ilieva*, A. M. Venezia, P. Petrova, G. Pantaleo, L. F. Liotta, R. Zanella, Z. Kaszkur, Y. Karakirova, T. Tabakova
P14: Impact of ceria loading on the preferential CO oxidation over gold catalysts on Y-doped CeO_2/Al_2O_3 supports	P. Petrova*, G. Pantaleo, R. Zanella, J. W. Sobczak, W. Lisowski, Z. Kaszkur, G. Munteanu, I. Yordanova, L. F. Liotta, A. M. Venezia, T. Tabakova, L. Ilieva
P15: Preparation, characterisation, and photocatalytic activity of boron-doped TiO_2-CNTs nanocomposites	V. B. Koli, J.-S. Kim*
P16: Cobalt oxide catalysts for deep oxidation of ethanol using plasma-aided deposition over stainless steel sieves	K. Jirátová*, P. Kšírová, M. Dvořáková, J. Balabánová, P. Topka, M. Čada, F. Kovanda
P17: Mechanochemically synthesised N-doped ZnO as catalysts for decolourisation of methyl orange and photodegradation of ciprofloxacin	N. G. Kostova*, M. Fabian, E. Dutkova, Y. Karakirova
P18: Modelling of ceria surface and nanoparticle models doped by Y^{3+} cations	H. A. Aleksandrov, I. Z. Koleva*, K. M. Neyman, G. N. Vayssilov
P19: DFT modelling of adsorption complexes of gas molecules on a Ni^{+}-exchanged ZSM-5 zeolite	I. Z. Koleva*, H. A. Aleksandrov, G. N. Vayssilov
P20: Density functional modelling of iron species in ZSM-5 zeolite	I. Z. Koleva*, H. A. Aleksandrov, W. Pantupho, S. Loiha, G. N. Vayssilov

P21: A facile synthesis of bimetallic nickel-ruthenium alloy nanoparticles and their catalytic performance in the dehydrogenation of morpholine borane as a new hydrogen storage material	B. Sundu*, T. Karaca, H. Can, Ö. Metin
P22: A DFT study on stability of Pt-Re surface alloys	A. Uzun*, B. S. Çağlayan, A. E. Aksoylu
P23: Cobalt ferrite modified with Hf(IV) as a catalyst for oxidation of ethyl acetate	M. Tsvetkov*, J. Zaharieva, G. Issa, M. Nedialkov, M. Milanova, Z. Cherkezova-Zheleva, T. Tsoncheva
P24: Sepiolite-supported nickel catalysts for hydrogen production by ammonia decomposition	S. F. Kurtoğlu*, S. Sarp, S. Soyer-Uzun, A. Uzun
P25: Copper catalysts supported on ordered mesoporous alumina-carbon composites in NO reduction with CO	N. Stoeva, I. Spassova*, P. Georgieva, M. Khristova
P26: IR spectroscopic characterisation of Hf-MOF-808	K. K. Chakarova*, M. Y. Mihaylov, K. I. Hadjiivanov, R. R. R. Prasad, P. A. Wright, M. L. Clarke
P27: Synthesis, characterisation, and catalytic behaviour of Zr- and Ti-modified Pd/La-Ce-Al catalysts for methane combustion in presence of H_2O and SO_2	R. Velinova*, B. Drenchev, G. Ivanov, M. Shipochka, P. Markov, D. Nihtianova, M. Shopska, D. Kovacheva, S .Todorova, A. Naydenov
P28: Mechanochemical synthesis and catalytic properties of calcium tungstate	M. Gancheva, R. Velinova*, R. Iordanova, A. Naydenov
P29: Influence of the methods of preparation on the structure and catalytic activity of silver-modified Beta	P. Konova*, Pl. Nikolov, N. Kumar, A. Naydenov
P30: Copper-modified coal ash zeolites as heterogeneous catalysts for VOCs oxidation	H. Lazarova*, S. Boycheva, D. Zgureva, M. Popova
P31: Selective reduction of NO by NH_3 over Fe_2O_3-promoted V_2O_5-WO_3/TiO_2 catalysts: significant suppression of N_2O formation	K. H. Yang, T. P. T. Nyguen, M. H. Kim*
P32: Hydrodesulphurisation catalysts deposited from NiMo complexes onto gamma-alumina prepared mechanochemically	L. Kaluža, K. Jirátová, G. Tyuliev*, D. Gulková, R. Palcheva, M. Koštejn, A. Spojakina
P33: Studies on the photocatalytic decomposition of water pollutant using TiO_2/reduced graphene oxide materials	A. Wanag*, E. Kusiak-Nejman, A. W. Morawski
P34: Naphthenes dehydroaromatisation and *n*-alkanes isomerisation over supported TMS catalysts	Al. A. Pimerzin*, A. I. Matveeva, A. A. Roganov, A. A. Pimerzin

P35: Effect of the magnesia in KCoMoS supported catalyst on selective hydrotreating of model FCC gasoline	Yu. V. Anashkin*, D. I. Ishutenko, P. A. Nikulshin, A. A. Pimerzin
P36: Distortions in IR spectra of adsorbed molecules caused by scattering	R. Novikov, A. Tsyganenko*
P37: From one-cation site model to binuclear cationic oxo-clusters in oxidative carbonylation of methanol over CuNaX zeolite	A. A. Rybakov, I. A. Bryukhanov, A. V. Larin*, G. M. Zhidomirov
P38: The use of ferroalloy production waste as a catalyst for oxidative process	A. K. Tleulesov, Zh. K. Shomanova, R. Z. Safarov*, V. V. Larichkin
P39: Nanosized K-modified transition metal sulphide catalysts for syngas conversion into alcohols and other oxygenates	V. V. Maximov*, V. S. Dorokhov, E. A. Permyakov, V. M. Kogan
P40: Green quaternisation of different N-heterocycles with 2-bromoethanol	S. Minkovska*, N. Burdzhiev, D. Radeva, T. Deligeorgiev
P41: CO and VOCs oxidation over alumina-supported Au-Cu-Mn catalysts: stability and poisoning resistance	E. Kolentsova*, D. Dimitrov, T. Tabakova, K. Ivanov
P42: Dry methane reforming on supported Ni-based catalysts promoted with Rh	S. Damyanova*, R. Palcheva, I. Shtereva, Y. Karakirova
P43: Photocatalytic degradation of paracetamol and chloramphenicol pharmaceuticals by Ln-modified ZnO photocatalysts	N. Kaneva, A. Bojinova*, K. Papazova, D. Dimitrov
P44: ANA-type zeolites synthesised from fly ash as CO_2 sorbent	B. Barbov, Yu. Kalvachev*
P45: Synthesis, characterisation, and catalytic properties of palladium nanoparticles stabilised by long alkyl chain N-heterocyclic carbene	M. E. Günay*, H. Arıcı, I. Zaier, Ö. Metin
P46: Highly efficient MgFe and Mg-Co-Fe mixed oxide catalysts for ammonia decomposition	S. Podila, H. Driss, S. F. Zaman, A. M. Ali, F. Bannani, A. A. Al-Zahrani, M. A. Daous, L. A. Petrov*
P47: Ammonia decomposition over citric acid cheated γ-Mo_2N and Ni_2Mo_3N catalysts	S. F. Zaman*, L. Jalaloso, A. A. Al-Zahrani, M. M. Daous, L. A. Petrov
P48: Ethyl benzene oxidative dehydrogenation to styrene on Al-B and Al-B-Sb catalysts	N. Pasupulety, A. A. Al-Zahrani, M. A. Daous, H. Driss, A. M. Ali, S. F. Zaman, L.A. Petrov*
P49: Hydrothermally stable support materials for the conversion of biomass	M. Schöneborn, P. Bussian, A. Malyschew*, T. Harmening, K. Heidkamp, M. Kuhn

P50: Catalytic methanation of atmospheric CO_2 for renewable power-to-gas	J. V. Veselovskaya*, O. V. Netskina, A. G. Okunev
P51: Aging of Cu/SSZ-13 for NH_3 SCR in mixed lean conditions	X. Auvray*, A. Grant, B. Lundberg, L. Olsson

17:45 **Sofia sightseeing tour (start at Park Hotel Moskva)**

Tuesday, 28th August 2018

08:30–19:30 **Registration and information**

Europe Hall

09:00–09:45	**IL6-Invited lecture**: Graphenes: a great challenge as support and catalysts for organic reactions	V. I. Parvulescu
09:45–10:30	**IL7-Invited lecture**: *Ab initio* quantum chemistry for understanding active site reactivity in zeolites	J. Sauer
10:30–11:00	**Coffee break**	
11:00–11:45	**IL8-Invited lecture**: Shape control of metal oxides for heterogeneous catalysis	W. Shen

Oral contributions

11:45–12:05	**O17**: Efficient production of 2,5-furandicarboxylic acid from an acetal form of 5-hydroxymethylfurfural with a CeO_2-supported Au catalyst	M. Kim, Y. Su, A. Fukuoka, E. J. M. Hensen, K. Nakajima*
12:05–12:25	**O18**: Probing acid sites in solid catalysts with pyridine UV-vis spectroscopy	M. E. Z. Velthoen*, S. Nab, B. M. Weckhuysen
12:30–13:30	**Lunch at Moskva restaurant**	
13:30–13:50	**O19**: R&D and industrial applications of SRIPT's ethylbenzene technology	W. Yang, Z. Wang*, H. Sun, B. Zhang
13:50–14:10	**O20**: Isobutanol conversion to propylene and butenes using catalysts based on MFI zeolites synthesised using microwave irradiation	A. A. Karavaev*, A. S. Loktev, A. G. Dedov
14:10–14:30	**O21**: Advantages of dual-bed system for co-processing a mixture of straight-run diesel and waste sunflower oil	A. N. Varakin, A. V. Mozhaev, A. A. Pimerzin, A. V. Fosler, P. A. Nikulshin*

14:30–14:50	**O22**: One-pot template-free synthesis of WO_3-SiO_2 nanomaterials in supercritical CO_2 as heterogeneous catalysts for alkene epoxidation	Y. Tao*, F. Picchioni, P. P. Pescarmona
14:50–15:10	**O23**: PtSn/γ-Al_2O_3 catalyst for direct propane dehydrogenation	A. M. Ali, M. B. Umar, S. Podila, N. Pasupulety, H. Driss, Y. Alhamed, A. A. Zahrani, M. A. Daous, L. A. Petrov*
15:10–15:30	**O24**: Reconstruction of oxide supports upon influence of Pd adlayers using supercell slab models	A. A. Rybakov, I. A. Bryukhanov, S. Todorova, R. Velinova, A. Naydenov, A. V. Larin*, G. M. Zhidomirov
15:30–15:50	**O25**: Ni stabilised in $La_2Zr_2O_7$: a robust catalyst for CO_2 recycling	E. le Saché*, L. Pastor-Pérez, D. Watson, A. Sepúlveda-Escribano, T. R. Reina
15:50–16:20	**Coffee break**	
16:20–16:40	**O26**: Thermal stability investigation on Mo/MCM-22 and Mo/ZSM-5 catalysts	Y. Liu*, F. Kooli, A. Borgna
16:40–17:00	**O27**: Influence of the composition and morphology of bulk catalysts synthesised from mixed Al_2O_3-supported $MoWS_2$ sulphides on their catalytic properties	A. V. Mozhaev*, M. S. Nikulshina, A. A. Sheldaisov-Mescheryakov, P. A. Nikulshin
17:00–17:20	**O28**: Coke oven gas hydrodesulphurisation	N. Kaisalo*, J. Kihlman, J. Palo, P. Jokimies
17:20–17:40	**O29**: Novel precursors in synthesis of KCoMoS catalysts for selective hydrotreating of FCC gasoline	D. I. Ishutenko*, Yu. V. Anashkin, P. A. Nikulshin
17:40–18:00	**O30**: The use of mixed SiW_1Mo_{11} heteropolyacid for preparation of NiMoW/Al_2O_3 sulphide catalyst for co-hydrotreating of light cycle oil with straight-run gas oil	M. Nikulshina*, A. Mozhaev, A. Kokliukhin, C. Lancelot, C. Lamonier, P. Minaev, P. Nikulshin
18:00–18:20	**O31**: Direct conversion of syngas to olefins over a bifunctional catalyst Cr-Zn mixed oxide/SAPO-34: tailoring activity and stability by varying the Cr/Zn ratio	V. P. Santos, A. C. Sandikci, G. Pollefeyt*, D. Nieskens, D. Yancey, A. Kirilin, A. Chojecki, A. Malek
18:20–18:40	**O32**: Effects of support composition on the performance of nickel catalysts in CO_2 methanation reaction	W. Gac*, G. Kolb, W. Zawadzki, M. Rotko, M. Greluk, G. Słowik, H. Pennemann, S. Neuberg

18:40–19:00	**O33**: Kinetics of syngas conversion to ethanol studied over silica-supported Rh catalysts	J. Bauer*, F. Schuster, R. Kraehnert, F. Rosowski
19:00–19:20	**O34**: Simultaneous methanation of carbon oxides on nickel-iron catalysts supported on ceria-doped gadolinia	P. Frontera, A. Macario, A. Malara*, V. Antonucci, V. Modafferi, P. L. Antonucci

Conference 3 Hall

Oral contributions

11:45–12:05	**O35**: Modelling of transition metal species and their complexes in the pores of zeolites	H. A. Aleksandrov*, I. Z. Koleva, G. N. Vayssilov
12:05–12:25	**O36**: Modelling of stability and catalytic behaviour of platinum species deposited on ceria surface and nanoparticles	G. N. Vayssilov*, H. A. Aleksandrov, I. Z. Koleva
12:30–13:30	**Lunch at Moskva restaurant**	
13:30–13:50	**O37**: Conversion of cellulose by heterogeneous catalysts	A. Fukuoka*, H. Kobayashi, A. Shrotri
13:50–14:10	**O38**: Glycerol etherification with isobutene for the production of fuel additives	Ö. D. Bozkurt*, N. Bağlar, S. Çelebi, A. Uzun
14:10–14:30	**O39**: Heterogeneous hydroconversion of biomass-derived γ-valerolactone over silica-supported Co catalyst	M. R. Mihályi*, G. Novodárszki, D. Deka, J. Valyon
14:30–14:50	**O40**: Low-temperature isomerisation-syncretisation conversion of a mixture of butane fraction with straight-run gasoline on anion-modified zeolite catalysts	M. T. Mamedova, S. I. Abasov*, S. B. Agaeva, D. B. Tagiev, A. A. Iskenderova, A. A. Imanova, E. S. Isayeva, A. R. Nasibova
14:50–15:10	**O41**: High temperature treatment of catalysts prepared by using the sol-gel method for higher activity of dimethyl ether direct synthesis	K. Takeishi*, T. Kishi
15:10–15:30	**O42**: Nonprecious bimetallic Ni-M/AlSBA-15 catalysts for semi-hydrogenation of phenylacetylene at near ambient condition	L. Yang*, Z. Zhou
15:30–15:50	**O43**: Base-free oxidation of 5-HMF derivatives by gold catalysts	Q. Yuan*, K. Hiemstra, T. G. Meinds, Z. Tang, L. Rohrbach, P. P. Pescarmona, H. J. Heeres, P. J. Deuss
15:50–16:20	**Coffee break**	

16:20–16:40	**O44**: Insights into surface phase formation and reactivity of monolayer V_2O_5-MoO_3/Al_2O_3 catalysts for oxidative dehydrogenation of propane	T. Kharlamova*, K. Timofeev, V. Svetlichnyi, O. Vodyankina
16:40–17:00	**O45**: Hydrolysis of cellulose on alumina-, silica-, and titania-supported heterogeneous catalysts	E. Kilic*, V. Degirmenci
17:00–17:20	**O46**: Study of CO_2 adsorption on a commercial CuO/ZnO/Al_2O_3 catalyst	M. Smyrnioti, T. Steriotis, T. Ioannides*
17:20–17:40	**O47**: Promotion of mesoporous nickel-alumina based catalysts by magnesium addition for reforming of waste gasification products	L. Karam*, N. El Hassan, F. Launay, P. Massiani
17:40–18:00	**O48**: Modifying the structure of red mud by simple treatments for high and stable performance in CO_x-free hydrogen production from ammonia	S. F. Kurtoğlu*, S. Soyer-Uzun, A. Uzun
18:00–18:20	**O49**: Utilisation of a MOF-derived highly dispersed Fe-based catalyst in ammonia decomposition reaction	Ö. Akarçay*, S. F. Kurtoğlu, A. Uzun
18:20–18:40	**O50**: Mesoporous silica materials with different pore sizes and geometries used as Ni hosts for the catalytic dry reforming of methane	O. Daoura*, S. Daher, M.-N. Kaydouh, N. El Hassan, P. Massiani, F. Launay, M. Boutros
18:40–19:00	**O51**: Structural investigation of Au, Pt, and Pd effects on the properties of Ni/Al_2O_3 as catalyst for methane dry reforming	D. Banerjee, G. Pantaleo, A. Longo, F. Puleo, C. Aprile, X. Collard, A. Martinez-Arias, L. F. Liotta*
19:00–19:20	**O52**: The effect of rapeseed oil and carbon monoxide on SRGO hydrotreating over sulphide CoMo/Al_2O_3 and NiMo/Al_2O_3 catalysts	E. N. Vlasova*, G. A. Bukhtiyarova, I. V. Deliy, P. V. Aleksandrov, A. A. Porsin, V. I. Bukhtiyarov

Wednesday, 29th August 2018

08:30–19:00 **Registration and information**

Europe Hall

09:00–09:45	**IL9-Invited lecture**: Enhancing the accessibility of active sites in TS-1-based catalysts for the epoxidation of biodiesel	R. Gläser

09:45–10:30	**IL10-Invited lecture**: Advanced researches on catalytic processing for air pollutant abatement	A. Giroir-Fendler
10:30–11:00	**Coffee break**	
11:00–11:45	**IL11-Invited lecture**: Oxygen activation and pathways in high-temperature catalytic oxidation	M. Sinev

Oral contributions

11:45–12:05	**O53**: Oxidative dehydrogenation of ethanol by modified OMS-2 catalysts	S. S. Dotsenko, V. A. Svetlichnyi, O. V. Vodyankina*
12:05–12:25	**O54**: On the structure and active sites of protected Au clusters supported on CeO_2	D. Pichugina*, N. Nikitina, M. Golosnaya, N. Kuz'menko
12:25–12:45	**O55**: Synthesis and catalytic performance of nanostructured Ag-doped lanthanum cobaltite catalytic thin films prepared by physical vapour deposition	A. Billard, I. Kalaitzidou, P. Vilasi, Ph. Vernoux, P. Briois*
12:45–13:45	**Lunch at Moskva restaurant**	
13:45–14:05	**O56**: Microemulsion synthesis of catalyst for hydrogen production *via* oxy-reforming and membrane reactor water-gas shift	F. Basile, S. Abate, A. Fasolini*, G. Centi
14:05–14:25	**O57**: Promoted Re/Al_2O_3 systems as sour water-gas shift catalysts	D. Nikolova*, R. Edreva-Kardjieva, H. Kolev, M. Gabrovska
14:25–14:45	**O58**: Magnetic and catalytic properties of Fe-Ni-Al oxide catalyst for hydrogenation of carbon dioxide	Sh. F. Tagiyeva*, E. H. Ismailov, E. E. Mamedov, R. J. Qasimov, N. M. Aliyeva
14:45–15:05	**O59**: Catalytic methanolysis of sodium borohydride	Ç. Çakanyıldırım
15:05–15:25	**O60**: Catalytic aqueous-phase reforming of Fischer-Tropsch derived alcohols for hydrogen production	I. Coronado*, M. Stekrova, R. Karinen, R. Puurunen, M. Reinikainen, J. Lehtonen
15:25–15:45	**O61**: Ni_xZn_{1-x} mixed ferrite-modified activated carbons from waste materials as catalysts for hydrogen production from methanol	T. Tsoncheva*, I. Genova, R. Ivanova, I. Spassova, D. Kovacheva, G. Issa, D. Paneva, D. Karashanova, M. Dimitrov, B. Georgieva, N. Velinov, I. Mitov, N. Petrov
15:45–16:15	**Coffee break**	

16:15–16:35	**O62**: Atomically dispersed copper on ceria nanostructures for CO oxidation	C. Papadopoulos, K. Kappis, J. Papavasiliou, J. Vakros, Y. Georgiou, Y. Deligiannakis, A. G. Chronis, M. M. Sigalas, G. Avgouropoulos*
16:35–16:55	**O63**: Gold nanoclusters dispersed on hydrothermally prepared copper-cerium oxide for preferential CO oxidation reaction	J. Papavasiliou
16:55–17:15	**O64**: Co_3O_4-MnO_x oxides supported on mesoporous and hierarchical macro-mesoporous silicas for CO and VOC oxidation	S. Todorova*, P. Gaudin, H. Kolev, A. Naydenov, B. Lebeau, A. Dozeva, D. Filkova, I. Ivaniva, L. Vidal, L. Michelin, J.-L. Blin
17:15–17:35	**O65**: Mesoporous nanostructured copper-titanium-cerium mixed oxides as catalysts for ethyl acetate oxidation and methanol decomposition	G. Issa*, A. Mileva, I. Genova, D. Kovacheva, G. Atanasova, J. Henych, J. Tolasz, V. Štengl, M. Dimitrov, T. Tsoncheva
17:35–17:55	**O66**: Mixed oxides of cerium and manganese as catalysts for total oxidation of ethyl acetate	M. Dimitrov*, R. Ivanova, G. Issa, D. Kovacheva, J. Henych, M. Kormunda, M. Slušná, J. Tolasz, V. Štengl, T. Tsoncheva
17:55–18:15	**O67**: Complete partial hydrogenation selectivity on a commercial supported nickel catalyst coated with ionic liquids	A. Jalal*, A. Uzun

Conference 3 Hall

Oral contributions

11:45–12:05	**O68**: Coal ash zeolites as heterogeneous catalysts for VOCs oxidation	S. Boycheva, D. Zgureva, H. Lazarova, M. Popova*
12:05–12:25	**O69**: Total oxidation of toluene over bimetallic (Cu, Fe) nanoporous silica catalysts	Á. Szegedi*, M. Popova, K. Lázár
12:25–12:45	**O70**: Pt/CeO_x/ZrO_x/Al_2O_3 ternary mixed oxide DeNO_x catalyst: surface chemistry and NO_x interaction	S. Andonova*, A. S. Ok, N. Drenchev, E. Ozensoy, K. Hadjiivanov
12:45–13:45	**Lunch at Moskva restaurant**	
13:45–14:05	**O71**: Polymeric dinuclear molybdenum(VI) complexes bearing α-aminoacid donor ligands as catalyst precursors for the selective oxyfunctionalisation of fine chemicals	I. Abdalghani, L. Biancalana, F. Ferella, F. Marchetti, M. Crucianelli*

14:05–14:25	**O72**: Catalytic performance and reaction pathways of Cu/SiO_2 and ZnO/SiO_2 for dehydrogenation of ethanol to acetaldehyde	M. Ohira, H. Liu, D. He, Y. Hirata, M. Sano, T. Suzuki, T. Miyake*
14:25–14:45	**O73**: Rh-catalysed hydrogenation of amino acids to bio-based amino alcohols: tackling challenging substrates and application to protein hydrolysates	A. Vandekerkhove*, L. Claes, F. De Schouwer, C. Van Goethem, I. F. J. Vankelecom, B. Lagrain, D. E. De Vos
14:45–15:05	**O74**: Molecular approaches in investigating the role of internal donors in heterogeneous Ziegler-Natta catalysts	A. K. Tomov*, M. Clarembeau, S. Bettonville, G. J. P. Britovsek
15:05–15:25	**O75**: Catalytic hydrogenation of CO_2 into valuable products on heterogeneous iron-based catalysts	N. D. Evdokimenko*, A. L. Kustov, K. O. Kim, L. M. Kustov
15:25–15:45	**O76**: Critical surface parameters for the oxidative coupling of methane over $Mn\text{-}Na\text{-}W/SiO_2$	N. S. Hayek*, N. S. Lucas, C. W. Damouny, O. M. Gazit
15:45–16:15	**Coffee break**	
16:15–16:35	**O77**: Promoting effects of Re, Cl, and alkali metals in silver-catalysed ethylene epoxidation	M. A. Salaev*, O. V. Vodyankina
16:35–16:55	**O78**: Transfer hydrogenolysis of aromatic ethers promoted by bimetallic Pd/Co catalyst	F. Mauriello, H. Ariga-Miwa, E. Paone*, R. Pietropaolo, S. Takakusagi, K. Asakura
16:55–17:15	**O79**: The use of polymer-stabilised ruthenium(0) nanoparticles as catalyst in hydrogen generation from morpholine borane: a new and cost-effective hydrogen storage medium	H. Can*, Ö. Metin
17:15–17:35	**O80**: Influence of the preparation method on the catalytic properties of $Mo\text{-}Fe\text{-}O/SiO_2$ catalysts in selective oxidation of 1,2-propanediol	D. Yu. Savenko*, N. Yu. Velieva, N. V. Dorofeeva, A. S. Savel'eva, V. A. Svetlichnyi, O. V. Vodyankina
17:35–17:55	**O81**: A seeded-growth synthesis of monodisperse Ag/Pd core-shell nano-particles and their catalytic performance in the dehydrogenation of ammonia-borane	M. S. Yilmaz*, T. Genez, Ö. Metin

Europe Hall

18:20–18:30	**Closing ceremony**	

Poster presentation

P37-From one-cation site model to binuclear cationic oxo-clusters in oxidative carbonylation of methanol over CuNaX zeolite

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Dimethylcarbonate (DMC) is one of green carbonylation/methylation agents and important fuel component with high oxygen content. The catalytic process of oxidative carbonylation on the Cu-form zeolites was studied herein as one of the possible alternatives instead of liquid-phase synthesis using corrosive solutions of CuCl [1,2]. Most authors accept that there are two steps in CH_3OH carbonylation, while the nature of intermediates is still under discussion. Zeroth kinetic order relative to oxygen concentration for DMC formation in three different Cu zeolites [3] points to probable Mars-van Krevelen mechanism in the opposite trend compared to liquid-state reaction in CuCl [1,2]. Regarding recently demonstrated oxidative activity of binuclear Cu_2O_x (x = 1, 2) [4] and trinuclear Cu_3O_3 clusters [5], participation of binuclear cationic $Cu(OH)_2Cu$ oxo-clusters has been admitted [6]. A three-stage carbonylation mechanism has been modelled using the PBE and PBEsol functionals within the projector augmented wave (PAW) method were performed with VASP [7]:

$$\{Cu^{+2}(OH)_2Cu^{+2}\}Z + CH_3OH \rightarrow \{Cu^{+2}(OCH_3)(OH)Cu^{+2}\}Z + H_2O \quad (1)$$

$$\{Cu^{+2}(OCH_3)(OH)Cu^{+2}\}Z + CH_3OH \rightarrow \{Cu^{+2}(OCH_3)_2Cu^{+2}\}Z + H_2O \quad (2)$$

$$\{Cu^{+2}(OCH_3)_2Cu^{+2}\}Z + CO \rightarrow \{Cu^{+2}(CH_3OCOOCH_3)Cu^{+2}\}Z \quad (3)$$

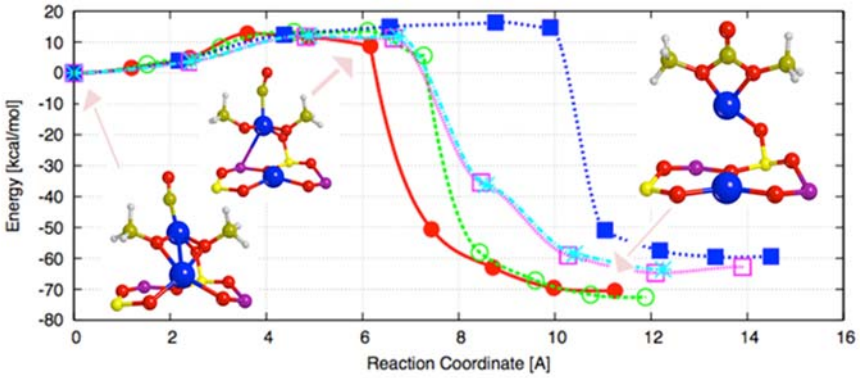

Fig. 1. Reaction coordinate (in Å) for CO attack over $Cu(OCH_3)_2Cu$ (3) in CuNaX obtained with different DFT functionals (PBE: closed circles, PBEsol: open circles) and using vdW corrections (PBE-D2: closed squares, PBE-D3(BJ): open squares, PBE-D3: stars) with periodic boundary conditions. The atomic colours are given in blue, red, yellow, magenta, olive, and grey for Cu, O, Si, Al, C, and H, respectively.

The results of the calculations using ciNEB algorithm [8] show that the step (3) is limiting one in agreement with experiment producing an activation barrier around 12–16 kcal/mol over CuNaX which is pretty close to the value 14.8 kcal/mol measured in CuY [3]. One believes that this route can be important for the Cu loadings when the concentration of binuclear copper clusters is essential.

Acknowledgement

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