

Publications 2012

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Research Papers in Periodicals (158)

Agarwala, H. ; Scherer, T. M. ; Maji, S. ; Mondal, T. K. ; Mobin, S. M. ; Fiedler, Jan ; Urbanos, F. A. ; Jimenez-Aparicio, R. ; Kaim, W. ; Lahiri, G. K. Correspondence of Ru^{III}Ru^{II} and Ru^{IV}Ru^{III} Mixed Valent States in a Small Dinuclear Complex. *Chemistry - A European Journal*, 2012, Roč. 18, č. 18, s. 5667-5675. ISSN 0947-6539.

Aguiar, A. L. ; San-Miguel, A. ; Barros, E. B. ; Kalbáč, Martin ; Machon, D. ; Kim, Y. A. ; Muramatsu, H. ; Endo, M. ; Souza Filho, A. G. Effects of intercalation and inhomogeneous filling on the collapse pressure of double-wall carbon nanotubes. *Physical Review. B*, 2012, Roč. 89, č. 19, s. 195410. ISSN 1098-0121.

Akhtar, M. N. ; Al-Yassir, N. ; Al-Khattaf, S. ; Čejka, Jiří. Aromatization of alkanes over Pt promoted conventional and mesoporous gallosilicates of MEL zeolite. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 61-72. ISSN 0920-5861.

Arenbergerová, M. ; Arenberger, P. ; Bednář, M. ; Kubát, Pavel ; Mosinger, Jiří. Light-activated nanofibre textiles exert antibacterial effects in the setting of chronic wound healing. *Experimental Dermatology*, 2012, Roč. 21, č. 8, s. 619-624. ISSN 0906-6705.

Bača, P. ; Micka, Karel ; Křivík, P. ; Tonar, K. ; Tošer, P. Investigation of the effect of mechanical pressure on the performance of negative lead accumulator electrodes during partial state of charge operation. *Journal of Power Sources*, 2012, Roč. 207, JUN 1 2012, s. 37-44. ISSN 0378-7753.

Bailleux, S. ; Zelinger, Zdeněk ; Beckers, H. ; Willner, H. ; Grigorová, E. High-resolution FTIR study of the CO stretching band v(4) of the fluoroformyloxyl radical, FCO₂. *Journal of Molecular Spectroscopy*, 2012, Roč. 278, AUG 2012, s. 11-16. ISSN 0022-2852.

Bandžuchová, L. ; Šelešovská, R. ; Navrátil, Tomáš ; Chýlková, J. ; Novotný, L. Voltammetric monitoring of electrochemical reduction of riboflavin using silver solid amalgam electrodes. *Electrochimica acta*, 2012, Roč. 75, July 2012, s. 316-324. ISSN 0013-4686.

Baše, Tomáš ; Bastl, Zdeněk ; Havránek, Vladimír ; Macháček, Jan ; Langecker, Jens ; Malina, Václav. Carboranedithiols: Building Blocks for Self-Assembled Monolayers on Copper Surfaces. *Langmuir*, 2012, Roč. 28, č. 34, s. 12518-12526. ISSN 0743-7463.

Bek, David ; Gawin, R. ; Grela, K. ; Balcar, Hynek. Ruthenium metathesis catalyst bearing chelating carboxylate ligand immobilized on mesoporous molecular sieve SBA-15. *Catalysis Communication*, 2012, Roč. 21, MAY 5 2012, s. 42-45. ISSN 1566-7367.

Beranová, Lenka ; Humpolíčková, Jana ; Sýkora, Jan ; Benda, Aleš ; Cwiklik, Lukasz ; Jurkiewicz, Piotr ; Gröbner, G. ; Hof, Martin. Effect of heavy water on phospholipid

membranes: experimental confirmation of molecular dynamics simulations. *Physical Chemistry Chemical Physics*, 2012, Roč. 14, č. 42, s. 14516-14522. ISSN 1463-9076.

Bhaskaran-Nair, Kiran ; Brabec, Jiří ; Apra, E. ; van Dam, H. J. J. ; Pittner, Jiří. Implementation of the multireference Brillouin-Wigner and Mukherjee's coupled cluster methods with non-iterative triple excitations utilizing reference-level parallelism. *Journal of Chemical Physics*, 2012, Roč. 137, č. 9, 094112. ISSN 0021-9606.

Bould, Jonathan ; Macháček, Jan ; Londesborough, Michael Geoffrey Stephen ; Macias, R. ; Kennedy, D. J. ; Bastl, Zdeněk ; Rupper, P. ; Baše, Tomáš. Decaborane Thiols as Building Blocks for Self-Assembled Monolayers on Metal Surfaces. *Inorganic Chemistry*, 2012, Roč. 51, č. 3, s. 1685-1694. ISSN 0020-1669.

Brabec, Jiří ; Bhaskaran-Neir, K. ; Govind, N. ; Pittner, Jiří. Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. *Journal of Chemical Physics*, 2012, Roč. 137, č. 17, s. 171101. ISSN 0021-9606.

Brabec, Jiří ; Pittner, Jiří ; van Dam, H. J. J. ; Apra, E. ; Kowalski, K. Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. *Journal of Chemical Theory and Computation*, 2012, Roč. 8, č. 2, s. 487-497. ISSN 1549-9618.

Brabec, Jiří ; Bhaskaran-Neir, K. ; Kowalski, K. ; Pittner, Jiří ; van Dam, H. J. J. Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthyne, and polycarbenes. *Chemical Physics Letters*, 2012, Roč. 542, 23 July, s. 128-133. ISSN 0009-2614.

Brabec, Jiří ; van Dam, H. J. J. ; Pittner, Jiří ; Kowalski, K. Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. *Journal of Chemical Physics*, 2012, Roč. 136, č. 12, s. 124102. ISSN 0021-9606.

Bubrin, M. ; Krafft, M. J. ; Steudle, L. ; Hübner, R. ; Field, J. S. ; Záliš, Stanislav ; Kaim, W. Structural Reassessment of [W(CO)(5)(TCNE)]: N (sigma) Coordination Instead of an Olefin (pi) Complex. *Organometallics*, 2012, Roč. 31, č. 17, s. 6305-6311. ISSN 0276-7333.

Bujdák, J. ; Danko, M. ; Chorvát Jr., D. ; Czímerová, A. ; Sýkora, Jan ; Lang, Kamil. Selective modification of layered silicate nanoparticle edges with fluorophores. *Applied Clay Science*, 2012, 65-66, SEP 2012, s. 152-157. ISSN 0169-1317.

Bulánek, R. ; Kalužová, A. ; Setnička, M. ; Zukal, Arnošt ; Čičmanec, P. ; Mayerová, Jana. Study of vanadium based mesoporous silicas for oxidative dehydrogenation of propane and n-butane. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 149-158. ISSN 0920-5861.

Ceausu-Velcescu, A. ; Pracna, Petr. The v3 + v5 combination band of DCF3: Modeling anharmonic and Coriolis interactions in a three-level system near 1700 cm⁻¹. *Journal of Molecular Spectroscopy*, 2012, Roč. 275, č. 276, s. 41-47. ISSN 0022-2852.

Cebecauer, Marek. Lipids and proteins in membranes: From in silico to in vivo. *Molecular Membrane Biology*, 2012, Roč. 29, č. 5, s. 115-117. ISSN 0968-7688.

Civiš, Svatopluk ; Ferus, Martin ; Kubelík, Petr ; Chernov, Vladislav E. ; Zanozina, Ekaterina M. Fourier transform infrared emission spectra of atomic rubidium: g- and h-states. *Journal of Physics B-Atomic Molecular and Optical Physics*, 2012, Roč. 45, č. 17, s. 175002. ISSN 0953-4075.

Civiš, Svatopluk ; Ferus, Martin ; Kubelík, Petr ; Jelínek, Petr ; Chernov, V. E. ; Knyazev, M. Yu. Laser ablation of CsI: time-resolved Fourier-transform infrared spectra of atomic cesium in the 800-8000 cm⁻¹ range. *Journal of the Optical Society of America. B*, 2012, Roč. 29, č. 5, s. 1112-1118. ISSN 0740-3224.

Civiš, Svatopluk ; Ferus, Martin ; Zukalová, Markéta ; Kubát, Pavel ; Kavan, Ladislav. Photochemistry and Gas-Phase FTIR Spectroscopy of Formic Acid Interaction with Anatase Ti₁₈O₂ Nanoparticles. *Journal of Physical Chemistry C*, 2012, Roč. 116, č. 20, s. 11200-11205. ISSN 1932-7447.

Civiš, Svatopluk ; Kubelík, Petr ; Ferus, Martin. Time-Resolved Fourier Transform Emission Spectroscopy of He/CH₄ in a Positive Column Discharge. *Journal of Physical Chemistry A*, 2012, Roč. 116, č. 12, s. 3137-3147. ISSN 1089-5639.

Čársky, Petr ; Čurík, Roman ; Varga, Š. Efficient evaluation of Coulomb integrals in a mixed Gaussian and plane-wave basis using the density fitting and Cholesky decomposition. *Journal of Chemical Physics*, 2012, Roč. 136, č. 11, s. 114105. ISSN 0021-9606.

Čejka, Jiří ; Centi, G. ; Pérez-Pariente, J. ; Roth, Wieslaw Jerzy. Zeolite-based materials for novel catalytic applications: Opportunities, perspectives and open problems. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 2-15. ISSN 0920-5861.

Das, A. K. ; Hübner, R. ; Sarkar, B. ; Fiedler, Jan ; Záliš, Stanislav ; Lahiri, G. K. ; Kaim, W. UV-vis-NIR and EPR characterisation of the redox series [MQ₃]₂₊,_{+,0,-2-}, M = Ru or Os, and Q = o-quinone derivative. *Dalton Transactions*, 2012, Roč. 41, č. 29, s. 8913-8921. ISSN 1477-9226.

Das, D. ; Scherer, T. M. ; Das, A. ; Mondal, T. K. ; Mobin, S. M. ; Fiedler, Jan ; Priego, J. L. ; Jiménez-Aparicio, R. ; Kaim, W. ; Lahiri, G. K. The intricate paramagnetic state of [Os(Q)(2)(bpy)](+), Q=4,6-di-tert-butyl-o-iminobenzoquinone. *Dalton Transactions*, 2012, Roč. 41, č. 38, s. 11675-11683. ISSN 1477-9226.

De Angelis, F. ; Vitillaro, G. ; Kavan, Ladislav ; Nazeeruddin, M. K. ; Grätzel, M. Modeling Ruthenium-Dye-Sensitized TiO₂ Surfaces Exposing the (001) or (101) Faces: A First-Principles Investigation. *Journal of Physical Chemistry C*, 2012, Roč. 116, č. 34, s. 18124-18131. ISSN 1932-7447.

de la Iglesia, O. ; Hrabánek, Pavel ; Zikánová, Arlette ; Kočířík, Milan. Study of the influence of gel composition in the synthesis of self-supported silicalite-1 layers. *Materials Letters*, 2012, Roč. 70, MAR 1 2012, s. 138-141. ISSN 0167-577X.

Dědeček, Jiří ; Sobálek, Zdeněk ; Wichterlová, Blanka. Siting and Distribution of Framework Aluminium Atoms in Silicon-Rich Zeolites and Impact on Catalysis. *Catalysis Reviews-Science and Engineering*, 2012, Roč. 54, č. 2, s. 135-223. ISSN 0161-4940.

Dědeček, Jiří ; Balgová, V. ; Pashková, Veronika ; Klein, Petr ; Wichterlová, Blanka. Synthesis of ZSM-5 Zeolites with Defined Distribution of Al Atoms in the Framework and Multinuclear MAS NMR Analysis of the Control of Al Distribution. *Chemistry of Materials*, 2012, Roč. 24, č. 16, s. 3231-3239. ISSN 0897-4756.

Deibel, N. ; Schweinfurth, D. ; Hohloch, S. ; Fiedler, Jan ; Sarkar, B. Donor-acceptor systems of Pt(II) and redox-induced reactivity towards small molecules. *Chemical Communications*, 2012, Roč. 48, č. 18, s. 2388-2390. ISSN 1359-7345.

Demel, Ondřej ; Kedžuch, S. ; Švaňa, Matěj ; Ten-no, S. ; Pittner, Jiří ; Noga, J. An explicitly correlated Mukherjee's state specific coupled cluster method: development and pilot applications. *Physical Chemistry Chemical Physics*, 2012, Roč. 14, č. 14, s. 4753-4763. ISSN 1463-9076.

Dohnalová, K. ; Fučíková, A. ; Umesh, Ch. P. ; Humpolíčková, Jana ; Paulusse, J. M. J. ; Valenta, J. ; Zuilhof, H. ; Hof, Martin ; Gregorkiewicz, T. Microscopic Origin of the Fast Blue-Green Luminescence of Chemically Synthesized Non-oxidized Silicon Quantum Dots. *Small*, 2012, Roč. 8, č. 20, s. 3185-3191. ISSN 1613-6810.

Drozd, A. ; Bubrin, M. ; Fiedler, Jan ; Záliš, Stanislav ; Kaim, W. (alpha-Diimine)tricarbonylhalorhenium complexes: the oxidation side. *Dalton Transactions*, 2012, Roč. 41, č. 3, s. 1013-1019. ISSN 1477-9226.

Durrell, A. C. ; Keller, G. E. ; Lam, Y. - Ch. ; Sýkora, Jan ; Vlček Jr., Antonín ; Gray, H. B. Structural Control of (1)A(2u)-to-(3)A(2u) Intersystem Crossing in Diplatinum(II,II) Complexes. *Journal of the American Chemical Society*, 2012, Roč. 134, č. 34, s. 14201-14207. ISSN 0002-7863.

Ehret, F. ; Bubrin, M. ; Hübner, R. ; Schweinfurth, D. ; Hartenbach, I. ; Záliš, Stanislav ; Kaim, W. Filling Gaps in the Series of Noninnocent Hetero-1,3-diene Chelate Ligands: Ruthenium Complexes of Redox-Active alpha-Azocarbonyl and alpha-Azothiocarbonyl Ligands RNNC(R')E, E = O or S. *Inorganic Chemistry*, 2012, Roč. 51, č. 11, s. 6237-6244. ISSN 0020-1669.

Fárník, Michal ; Poterya, Viktoriya ; Kočíšek, Jaroslav ; Fedor, Juraj ; Slavíček, P. Short review on the acetylene photochemistry in clusters: photofragment caging and reactivity. *Molecular Physics*, 2012, Roč. 110, 21-22, s. 2817-2828. ISSN 0026-8976.

Ferus, Martin ; Civiš, Martin ; Mládek, Arnošt ; Šponer, Jiří ; Juha, Libor ; Šponer, Judit E. On the Road from Formamide Ices to Nucleobases: IR-Spectroscopic Observation of a Direct Reaction between Cyano Radicals and Formamide in a High-Energy Impact Event. *Journal of the American Chemical Society*, 2012, Roč. 134, č. 51, s. 20788-20796. ISSN 0002-7863.

Fišer, J. ; Polák, Rudolf. A theoretical study of spectroscopy and metastability of the CN₂⁺ dication. *Chemical Physics*, 2012, Roč. 392, č. 1, s. 55-62. ISSN 0301-0104.

Forrage, J. ; Peltier, C. ; Perruchot, Ch. ; Takemoto, Y. ; Teki, Y. ; Bedioui, F. ; Marvand, V. ; Dupeyre, G. ; Pospíšil, Lubomír ; Adamo, C. ; Hromadová, Magdaléna ; Ciofini, I. ; Lainé, P. P. Single-Step versus Stepwise Two-Electron Reduction of Polyarylpyridiniums: Insights

from the Steric Switching of Redox Potential Compression. *Journal of the American Chemical Society*, 2012, Roč. 134, č. 5, s. 2691-2705. ISSN 0002-7863.

Frank, Otakar ; Bouša, Milan ; Riaz, I. ; Jalil, R. ; Novoselov, K. S. ; Tsoukleri, G. ; Parthenios, J. ; Kavan, Ladislav ; Papagelis, K. ; Gallois, C. Phonon and Structural Changes in Deformed Bernal Stacked Bilayer Graphene. *Nano Letters*, 2012, Roč. 12, č. 2, s. 687-693. ISSN 1530-6984.

Frank, Otakar ; Zukalová, Markéta ; Lásková, Barbora ; Kürti, J. ; Koltai, J. ; Kavan, Ladislav. Raman spectra of titanium dioxide (anatase, rutile) with identified oxygen isotopes (16, 17, 18). *Physical Chemistry Chemical Physics*, 2012, Roč. 14, č. 42, s. 14567-14572. ISSN 1463-9076.

Fryčák, P. ; Jirkovský, Jaromír ; Ranc, V. ; Bednář, P. ; Havlíček, Vladimír ; Lemr, Karel. Secondary processes in atmospheric pressure chemical ionization-ion trap mass spectrometry: a case study of orotic acid. *Journal of Mass Spectrometry*, 2012, Roč. 47, č. 6, s. 720-726. ISSN 1076-5174.

Fryčová, Marie ; Sysel, P. ; Kočířík, Milan ; Brabec, Libor ; Hrabánek, Pavel ; Prokopová, Olga ; Bernauer, B. ; Zikánová, Arlette. Mixed matrix membranes based on 3-aminopropyltriethoxysilane endcapped polyimides and silicalite-1. *Journal of Applied Polymer Science*, 2012, Roč. 124, SI 1, E233-E240. ISSN 0021-8995.

Gál, Miroslav ; Kolivoška, Viliam ; Kavan, Ladislav ; Bulíčková, Jana ; Pospíšil, Lubomír ; Hromadová, Magdaléna ; Zukalová, Markéta ; Sokolová, Romana ; Kielar, F. On the Stability of Fullerene C₆₀ in Aqueous Medium. *Fullerenes, Nanotubes, and Carbon Nanostructures*, 2012, Roč. 20, č. 8, s. 737-742. ISSN 1536-383X.

Gil, B. ; Marszalek, B. ; Adamski, A. ; Olejniczak, Z. ; Kubů, Martin ; Čejka, Jiří. On the location of iron and aluminium atoms in thermally activated AlMCM-58 and FeMCM-58 zeolites. *Microporous and Mesoporous Materials*, 2012, Roč. 151, MAR 15 2012, s. 339-345. ISSN 1387-1811.

Gilchrist, F. J. ; Razavi, C. ; Webb, A. K. ; Jones, A.M. ; Španěl, Patrik ; Smith, D. ; Lenney, W. An investigation of suitable bag materials for the collection and storage of breath samples containing hydrogen cyanide. *Journal of Breath Research*, 2012, Roč. 6, č. 3, 036004. ISSN 1752-7155.

Gilchrist, F. J. ; Sims, H. ; Alcock, A. ; Belcher, J. ; Jones, A.M. ; Smith, D. ; Španěl, Patrik ; Webb, A. K. ; Lenney, W. Quantification of hydrogen cyanide and 2-aminoacetophenone in the headspace of *Pseudomonas aeruginosa* cultured under biofilm and planktonic conditions. *Analytical Methods: advancing methods and applications*, 2012, Roč. 4, č. 11, s. 3661-3665. ISSN 1759-9660.

Glodic, P. ; Kartakoullis, A. ; Fárník, Michal ; Samartzis, P. C. ; Kitsopoulos, T. N. Driving photochemistry by clustering: The ICl-Xe case. *Journal of Chemical Physics*, 2012, Roč. 137, č. 15, s. 154306. ISSN 0021-9606.

Grajciar, L. ; Čejka, Jiří ; Zukal, Arnošt ; Areán, C. O. ; Turnes Palomino, G. ; Nachtigall, P. Controlling the Adsorption Enthalpy of CO₂ in Zeolites by Framework Topology and Composition. *ChemSusChem*, 2012, Roč. 5, č. 10, s. 2011-2022. ISSN 1864-5631.

Guerin, V. M. ; Rathouský, Jiří ; Pauperté, T. Electrochemical design of ZnO hierarchical structures for dye-sensitized solar cells. *Solar Energy Materials and Solar Cells*, 2012, Roč. 102, JUL 2012, s. 8-14. ISSN 0927-0248.

Hanková, V. ; Slováková, E. ; Zedník, J. ; Vohlídal, J. ; Sivková, R. ; Balcar, Hynek ; Zukal, Arnošt ; Brus, Jiří ; Sedláček, J. Polyacetylene-Type Networks Prepared by Coordination Polymerization of Diethynylarenene: New Type of Microporous Organic Polymers. *Macromolecular Rapid Communications*, 2012, Roč. 33, č. 2, s. 158-163. ISSN 1022-1336.

Havlík, A. ; Lamač, Martin ; Pinkas, Jiří ; Padělková, Z. ; Růžička, A. ; Gyepes, Robert ; Horáček, Michal. Synthesis, structure, and fluxional behaviour of highly-substituted group 4 cyclopentadienyl arylamine complexes. *Journal of Organometallic Chemistry*, 2012, Roč. 719, November, s. 64-73. ISSN 0022-328X.

Herman, Zdeněk ; Žabka, Ján ; Pysanenko, Andriy. Survival probability of slow ions colliding with room-temperature and heated surfaces of beryllium. *Molecular Physics*, 2012, Roč. 110, 15-16, s. 1669-1673. ISSN 0026-8976.

Heydová, Radka ; Gindensperger, E. ; Romano, R. ; Sýkora, Jan ; Vlček Jr., Antonín ; Záliš, Stanislav ; Daniel, CH. Spin–Orbit Treatment of UV–vis Absorption Spectra and Photophysics of Rhenium(I) Carbonyl–Bipyridine Complexes: MS-CASPT2 and TD-DFT Analysis. *Journal of Physical Chemistry A*, 2012, Roč. 116, č. 46, s. 11319-11329. ISSN 1089-5639.

Hübner, R. ; Sarkar, B. ; Fiedler, Jan ; Záliš, Stanislav ; Kaim, W. Metal(IV) Complexes [M(LN,O,S)2]n (M = Ru, Os) of a Redox-Active o-Amidophenolate Ligand (LN,O,S)2-with Coordinating Thioether Appendix. *European Journal of Inorganic Chemistry*, 2012, Roč. 2012, č. 11, s. 3569-3576. ISSN 1434-1948.

Chlubná, Pavla ; Roth, W. J. ; Zukal, Arnošt ; Kubů, Martin ; Pavlatová, Jana. Pillared MWW zeolites MCM-36 prepared by swelling MCM-22P in concentrated surfactant solutions. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 35-42. ISSN 0920-5861.

Jurkiewicz, Piotr ; Olżyńska, Agnieszka ; Cwiklik, Lukasz ; Conte, E. ; Jungwirth, Pavel ; Megli, F. M. ; Hof, Martin. Biophysics of lipid bilayers containing oxidatively modified phospholipids: Insights from fluorescence and EPR experiments and from MD simulations. *Biochimica Et Biophysica Acta-Biomembranes*, 2012, Roč. 1818, č. 10, s. 2388-2402. ISSN 0005-2736.

Jurkiewicz, Piotr ; Cwiklik, Lukasz ; Jungwirth, Pavel ; Hof, Martin. Lipid hydration and mobility: An interplay between fluorescence solvent relaxation experiments and molecular dynamics simulations. *Biochimie*, 2012, Roč. 94, č. 1, s. 26-32. ISSN 0300-9084.

Jurkiewicz, Piotr ; Cwiklik, Lukasz ; Vojtíšková, Alžběta ; Jungwirth, Pavel ; Hof, Martin. Structure, dynamics, and hydration of POPC/POPS bilayers suspended in NaCl, KCl, and

CsCl solutions. *Biochimica Et Biophysica Acta-Biomembranes*, 2012, Roč. 1818, č. 3, s. 609-616. ISSN 0005-2736.

Kalbáč, Martin ; Frank, Otakar ; Kavan, Ladislav. Effects of Heat Treatment on Raman Spectra of Two-Layer 12C/13C Graphene. *Chemistry - A European Journal*, 2012, Roč. 18, č. 43, s. 13877-13884. ISSN 0947-6539.

Kalbáč, Martin ; Frank, Otakar ; Kong, J. ; Sanchez-Yamagishi, J. ; Watanabe, K. ; Taniguchi, T. ; Jarillo-Herrero, P. ; Dresselhaus, M. S. Large Variations of the Raman Signal in the Spectra of Twisted Bilayer Graphene on a BN Substrate. *Journal of Physical Chemistry Letters*, 2012, Roč. 3, č. 6, s. 796-799. ISSN 1948-7185.

Kalbáč, Martin ; Kong, J. ; Dresselhaus, M. S. Raman Spectroscopy as a Tool to Address Individual Graphene Layers in Few-Layer Graphene. *Journal of Physical Chemistry C*, 2012, Roč. 116, č. 35, s. 19046-19050. ISSN 1932-7447.

Kalbáč, Martin ; Kong, J. ; Kavan, Ladislav ; Dresselhaus, M. S. Raman spectroscopy of isotopically labeled two-layer graphene. *Physica Status Solidi B-Basic Solid State Physics*, 2012, Roč. 249, č. 12, s. 2500-2502. ISSN 0370-1972.

Kalbáč, Martin ; Frank, Otakar ; Kavan, Ladislav. The control of graphene double-layer formation in copper-catalyzed chemical vapor deposition. *Carbon*, 2012, Roč. 50, č. 10, s. 3682-3687. ISSN 0008-6223.

Kalbáčová, M. ; Brož, A. ; Kalbáč, Martin. Influence of the fetal bovine serum proteins on the growth of human osteoblast cells on graphene. *Journal of Biomedical Materials Research. Part A*, 2012, 100A, č. 11, s. 3001-3007. ISSN 1549-3296.

Kämper, S. ; Paretzki, A. ; Fiedler, Jan ; Záliš, Stanislav ; Kaim, W. Solar Cell Sensitizer Models [Ru(bpy-R)(2)(NCS)(2)] Probed by Spectroelectrochemistry. *Inorganic Chemistry*, 2012, Roč. 51, č. 4, s. 2097-2104. ISSN 0020-1669.

Kapusta, Peter ; Macháň, Radek ; Benda, A. ; Hof, Martin. Fluorescence Lifetime Correlation Spectroscopy (FLCS): Concepts, Applications and Outlook. *International Journal of Molecular Sciences*, 2012, Roč. 13, č. 10, s. 12890-12910. ISSN 1422-0067.

Kárászová, Magda ; Vejražka, Jiří ; Veselý, Václav ; Friess, K. ; Randová, A. ; Hejtmánek, Vladimír ; Brabec, Libor ; Izák, Pavel. A Water-Swollen Thin Film Composite Membrane for Effective Upgrading of Raw Biogass by Methane. *Separation and Purification Technology*, 2012, Roč. 89, MAR 22, s. 212-216. ISSN 1383-5866.

Kavan, Ladislav. Electrochemistry of titanium dioxide: some aspects and highlights. *Chemical Record*, 2012, Roč. 12, č. 1, s. 131-142. ISSN 1527-8999.

Kavan, Ladislav. Nanomaterials based on carbon and Ti(IV) oxides: some aspects of their electrochemistry. *International Journal of Nanotechnology*, 2012, Roč. 9, 8/9, s. 652-679. ISSN 1475-7435.

Kavan, Ladislav ; Yum, J. H. ; Graetzel, M. Optically Transparent Cathode for Co(III/II) Mediated Dye-Sensitized Solar Cells Based on Graphene Oxide. *ACS Applied Materials and Interfaces*, 2012, Roč. 4, č. 12, s. 6998-7005. ISSN 1944-8244.

Khabiri, Morteza ; Roeselová, Martina ; Cwiklik, Lukasz. Properties of oxidized phospholipid monolayers: An atomistic molecular dynamics study. *Chemical Physics Letters*, 2012, 519-520, 5 Jan, s. 93-99. ISSN 0009-2614.

Kirakci, Kaplan ; Kubát, Pavel ; Dušek, Michal ; Fejfarová, Karla ; Šícha, Václav ; Mosinger, Jiří ; Lang, Kamil. A Highly Luminescent Hexanuclear Molybdenum Cluster - A Promising Candidate toward Photoactive Materials. *European Journal of Inorganic Chemistry*, 2012, Roč. 2012, č. 19, s. 3107-3111. ISSN 1434-1948.

Klíma, Jiří ; Polášek, Miroslav ; Ludvík, Jiří ; Urban, Jiří. Reaction of Phthalaldehyde with Aminoethanol under Different Conditions: Products and Mechanisms of Their Formation. *Journal of Heterocyclic Chemistry*, 2012, Roč. 49, č. 5, s. 1202-1209. ISSN 0022-152X.

Kolivoška, Viliam ; Gál, Miroslav ; Hromadová, Magdaléna ; Lachmanová, Štěpánka ; Tarábková, Hana ; Janda, Pavel ; Pospíšil, Lubomír ; Morovská Turoňová, A. Bovine serum albumin film as a template for controlled nanopancake and nanobubble formation: In situ atomic force microscopy and nanolithography study. *Colloids and Surfaces B-Biointerfaces*, 2012, Roč. 94, JUN 1 2012, s. 213-219. ISSN 0927-7765.

Kovalenko, Alexander ; Petráková, Vladimíra ; Ashcheulov, Petr ; Záliš, Stanislav ; Nesladek, M. ; Kraus, I. ; Kratochvílová, Irena. Parameters affecting the luminescence of nanodiamond particles: Quantum chemical calculations. *Physica Status Solidi. A*, 2012, Roč. 209, č. 9, s. 1769-1773. ISSN 1862-6300.

[http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1862-6319/earlyview](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1862-6319/earlyview)

Krabáč, Lubomír ; Klementová, Mariana ; Šubrt, Jan ; Fajgar, Radek ; Kupčík, Jaroslav ; Bastl, Zdeněk ; Stuchlíková, The-Ha ; Dřínek, Vladislav. Preparation of Si/O/C Nanotubes Using Ge Nanowires as Template. *Journal of Analytical and Applied Pyrolysis*, 2012, Roč. 97, SEP, s. 94-98. ISSN 0165-2370.

Křivík, P. ; Micka, Karel ; Bača, P. ; Tonar, K. ; Tošer, P. Effect of additives on the performance of negative lead-acid battery electrodes during formation and partial state of charge operation. *Journal of Power Sources*, 2012, Roč. 209, JUL 1 2012, s. 15-19. ISSN 0378-7753.

Kubišta, Jiří ; Civiš, Martin ; Španěl, Patrik ; Civiš, Svatopluk. Combining Fourier transform nuclear quadrupole resonance (FT-NQR) spectroscopy and mass spectrometry (MS) to study the electronic structure of titanocene dichlorides. *Analyst*, 2012, Roč. 137, č. 6, s. 1338-1342. ISSN 0003-2654.

Kumar, S. ; Huang, J. ; Cushnir, J. R. ; Španěl, Patrik ; Smith, D. Selected Ion Flow Tube-MS Analysis of Headspace Vapor from Gastric Content for the Diagnosis of Gastro-Esophageal Cancer. *Analytical Chemistry*, 2012, Roč. 84, č. 21, s. 9550-9557. ISSN 0003-2700.

Kundu, T. ; Schweinfurth, D. ; Sarkar, B. ; Mondal, T. K. ; Fiedler, Jan ; Mobin, S. M. ; Puranik, V. G. ; Kaim, W. ; Lahiri, G. K. Strong metal-metal coupling in mixed-valent

intermediates $[\text{Cl}(\text{L})\text{Ru}(\mu\text{-tppz})\text{Ru}(\text{L})\text{Cl}]^+$, L = beta-diketonato ligands, tppz=2,3,5,6-tetrakis(2-pyridyl)pyrazine. *Dalton Transactions*, 2012, Roč. 41, č. 43, s. 13429-13440. ISSN 1477-9226.

Kurfiřtová, Lenka ; Seo, Y. - K. ; Hwang, Y. K. ; Chang, J. - S. ; Čejka, Jiří. High activity of iron containing metal-organic-framework in acylation of p-xylene with benzoyl chloride. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 85-90. ISSN 0920-5861.

Langmaier, Jan ; Samec, Zdeněk ; Samcová, E. ; Tůma, P. Transfer of heparin polyion across a polarized water/ionic liquid membrane interface. *Electrochemistry Communications*, 2012, Roč. 24, OCT 2012, s. 25-27. ISSN 1388-2481.

Lásková, Barbora ; Zukalová, Markéta ; Kavan, Ladislav ; Chou, A. ; Liska, P. ; Wei, Z. ; Bin, L. ; Kubát, Pavel ; Ghadiri, E. ; Moser, J. E. ; Grätzel, M. Voltage enhancement in dye-sensitized solar cell using (001)-oriented anatase TiO₂ nanosheets. *Journal of Solid State Electrochemistry*, 2012, Roč. 16, č. 9, s. 2993-3001. ISSN 1432-8488.

Lengyel, Jozef ; Pysanenko, Andriy ; Kočíšek, Jaroslav ; Poterya, Viktoriya ; Pradzynski, Ch. C. ; Zeuch, T. ; Slavíček, Petr ; Fárník, Michal. Nucleation of Mixed Nitric Acid-Water Ice Nanoparticles in Molecular Beams that Starts with a HNO₃ Molecule. *Journal of Physical Chemistry Letters*, 2012, Roč. 3, č. 21, s. 3096-3101. ISSN 1948-7185.

Lengyel, Jozef ; Rimarčík, J. ; Vagánek, A. ; Fedor, J. ; Lukeš, V. ; Klein, E. Oxidation of sterols: Energetics of C-H and O-H bond cleavage. *Food Chemistry*, 2012, Roč. 133, č. 4, s. 1435-1440. ISSN 0308-8146.

Lengyel, Jozef ; Kočíšek, Jaroslav ; Poterya, Viktoriya ; Pysanenko, Andriy ; Svrčková, Pavla ; Fárník, Michal ; Zaouris, D. K. ; Fedor, J. Uptake of atmospheric molecules by ice nanoparticles: Pickup cross sections. *Journal of Chemical Physics*, 2012, Roč. 137, č. 3, 034304. ISSN 0021-9606.

Lhotáková, Y. ; Plíštil, L. ; Morávková, A. ; Kubát, Pavel ; Lang, Kamil ; Forstová, J. ; Mosinger, J. Virucidal Nanofiber Textiles Based on Photosensitized Production of Singlet Oxygen. *PLoS ONE*, 2012, Roč. 7, č. 11, e49226. ISSN 1932-6203.

Linseis, M. ; Záliš, Stanislav ; Zabel, M. ; Winter, R. F. Ruthenium Stilbenyl and Diruthenium Distyrylethene Complexes: Aspects of Electron Delocalization and Electrocatalyzed Isomerization of the Z-Isomer. *Journal of the American Chemical Society*, 2012, Roč. 134, č. 40, s. 16671-16692. ISSN 0002-7863.

Lis, M. ; Pintal, L. ; Swiatek, J. ; Cwiklik, Lukasz. GPU-Based Massive Parallel Kawasaki Kinetics in the Dynamic Monte Carlo Simulations of Lipid Nanodomains. *Journal of Chemical Theory and Computation*, 2012, Roč. 8, č. 11, s. 4758-4765. ISSN 1549-9618.

Liu, Y. ; Štefanić, G. ; Rathouský, Jiří ; Hayden, O. ; Bein, T. ; Fattakhova-Rohlfing, D. Assembly of mesoporous indium tin oxide electrodes from nano-hydroxide building blocks. *Chemical Science*, 2012, Roč. 3, č. 7, s. 2367-2374. ISSN 2041-6520.

Londesborough, Michael Geoffrey Stephen ; Hnyk, Drahomír ; Bould, Jonathan ; Serrano-Andrés, L. ; Sauri, V. ; Oliva, J. M. ; Kubát, Pavel ; Polívka, T. ; Lang, Kamil. Distinct

Photophysics of the Isomers of B18H22 Explained. *Inorganic Chemistry*, 2012, Roč. 51, č. 3, s. 1471-1479. ISSN 0020-1669.

Lyutakov, O. ; Huttel, I. ; Tůma, J. ; Kalbáč, Martin ; Janoušek, M. ; Šimek, P. ; Svorcik, V. Ordered graphene strips onto polymer backing prepared by laser scanning. *Applied Physics Letters*, 2012, Roč. 101, č. 17, s. 173102. ISSN 0003-6951.

Metelková, R. ; Tobrman, T. ; Kvapilová, Hana ; Hoskovicová, I. ; Ludvík, Jiří. Synthesis, characterization and electrochemical investigation of hetaryl chromium(0) aminocarbene complexes. *Electrochimica acta*, 2012, Roč. 82, SI, s. 470-477. ISSN 0013-4686.

Mills, A. ; O'Rourke, Ch. ; Kalousek, Vít ; Rathouský, Jiří. Adsorption and photocatalytic and photosensitised bleaching of acid orange 7 on multilayer mesoporous films of TiO₂. *Journal of Hazardous Materials*, 2012, Roč. 211, SI, s. 182-187. ISSN 0304-3894.

Mrázová, K. ; Navrátil, Tomáš ; Pelcová, D. Consequences of Ingestions of Potentially Corrosive Cleaning Products, One-Year Follow-Up. *International Journal of Electrochemical Science*, 2012, Roč. 7, č. 3, s. 1734-1748. ISSN 1452-3981.

 <http://www.electrochemsci.org/papers/vol7/7031734.pdf>

Müller, V. ; Haase, F. ; Rathouský, Jiří ; Fattakhova-Rohlfing, D. Surface functionalization of mesoporous antimony doped tin oxide by metalorganic reaction. *Materials Chemistry and Physics*, 2012, Roč. 137, č. 1, s. 207-212. ISSN 0254-0584.

Müller, V. ; Haase, F. ; Rathouský, Jiří ; Fattakhova-Rohlfing, D. Surface functionalization of mesoporous antimony doped tin oxide by metalorganic reaction. *Materials Chemistry and Physics*, 2012, Roč. 137, č. 1, s. 207-212. ISSN 0254-0584.

Nachtigall, P. ; Grajciar, L. ; Pérez-Pariente, J. ; Pinar, A. B. ; Zukal, Arnošt ; Čejka, Jiří. Control of CO(2) adsorption heats by the Al distribution in FER zeolites: effect of synthesis conditions. *Physical Chemistry Chemical Physics*, 2012, Roč. 14, č. 3, s. 1117-1120. ISSN 1463-9076.

Olejník, R. ; Padělková, Z. ; Horáček, Michal ; Růžička, A. Structure of beta-diketiminates and beta-aminoketones made from anisidines or chloroanilines: tin and lithium complexes. *Main Group Metal Chemistry*, 2012, Roč. 35, 1-2, s. 13-27. ISSN 0334-7575.

Olivares, A. ; Dryahina, Kseniya ; Španěl, Patrik ; Flores, M. Rapid detection of lipid oxidation in beef muscle packed under modified atmosphere by measuring volatile organic compounds using SIFT-MS. *Food Chemistry*, 2012, Roč. 135, č. 3, s. 1801-1808. ISSN 0308-8146.

Pelcová, D. ; Fenclová, Z. ; Vlčková, Š. ; Lebedová, J. ; Syslová, K. ; Pecha, O. ; Běláček, J. ; Navrátil, Tomáš ; Kuzma, Marek ; Kačer, P. Leukotrienes B4, C4, D4 and E4 in the Exhaled Breath Condensate (EBC), Blood and Urine in Patients with Pneumoconiosis. *Industrial Health*, 2012, Roč. 50, č. 4, s. 299-306. ISSN 0019-8366.

Pérez-Mayoral, E. ; Musilová, Zuzana ; Gil, B. ; Marszalek, B. ; Položij, M. ; Nachtigall, P. ; Čejka, Jiří. Synthesis of quinolines via Friedlander reaction catalyzed by CuBTC metal-

organic-framework. *Dalton Transactions*, 2012, Roč. 41, č. 14, s. 4036-4044. ISSN 1477-9226.

Pick, Štěpán. Density-functional study of the compressed $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ -CO overlayer on the ferromagnetic Co(0001) surface. *Surface Science*, 2012, Roč. 606, 7-8, s. 692-696. ISSN 0039-6028.

Pinkas, Jiří ; Císařová, Ivana ; Gyepes, Robert ; Kubišta, Jiří ; Horáček, Michal ; Mach, Karel. Ethene Complexes of Bulky Titanocenes, Their Thermolysis, and Their Reactivity toward 2-Butyne. *Organometallics*, 2012, Roč. 31, č. 15, s. 5478-5493. ISSN 0276-7333.

Pinkas, Jiří ; Císařová, I. ; Karban, Jindřich ; Schraml, Jan ; Sýkora, Jan. Identification of branched oligosilanes in the phenylsilane dehydrocoupling reaction. *Journal of Organometallic Chemistry*, 2012, Roč. 710, JUL 1 2012, s. 20-25. ISSN 0022-328X.

Plasser, F. ; Granucci, G. ; Pittner, Jiří ; Barbatti, M. ; Persico, M. ; Lischka, H. Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, 2012, Roč. 137, č. 22, 22A514. ISSN 0021-9606.

Pluhařová, Eva ; Ončák, M. ; Seidel, R. ; Schroeder, C. ; Schroeder, W. ; Winter, B. ; Bradforth, S. E. ; Jungwirth, Pavel ; Slavíček, Petr. Transforming Anion Instability into Stability: Contrasting Photoionization of Three Protonation Forms of the Phosphate Ion upon Moving into Water. *Journal of Physical Chemistry B*, 2012, Roč. 116, č. 44, s. 13254-13264. ISSN 1520-6106.

Pola, Josef ; Urbanová, Markéta ; Pokorná, Dana ; Bakardjieva, Snejana ; Šubrt, Jan ; Bastl, Zdeněk ; Gondal, M.A. ; Masoudi, H.M. IR Laser Photodeposition of a-Fe/Si Films Developing Nanograins of Ferrisilicate, Iron Disilicide and Rare Hexagonal Iron upon Annealing. *Dalton Transactions*, 2012, Roč. 41, č. 6, s. 1727-1733. ISSN 1477-9226.

Pola, Josef ; Gondal, M.A. ; Urbanová, Markéta ; Pokorná, Dana ; Masoudi, H.M. ; Bakardjieva, Snejana ; Bastl, Zdeněk ; Šubrt, Jan ; Siddiqui, M.N. Laser Photochemical Deposition of Magnetite Nanograins in a-Fe/C/O Composite: High-Pressure Metal Oxide Polymorph Surviving Ambient Conditions. *Journal of Photochemistry and Photobiology A-Chemistry*, 2012, Roč. 243, SEP 1, s. 33-40. ISSN 1010-6030.

Poterya, Viktoriya ; Šištík, L. ; Slavíček, Petr ; Fárník, Michal. Hydrogen bond dynamics in the excited states: Photodissociation of phenol in clusters. *Physical Chemistry Chemical Physics*, 2012, Roč. 14, č. 25, s. 8936-8944. ISSN 1463-9076.

Pracna, Petr ; Pretkowski, T. ; Lodyga, W. ; Kreglewski, M. High-resolution infrared spectroscopy of the $v_2 = v_6 = 1$ combination level of DCF₃. *Journal of Molecular Spectroscopy*, 2012, Roč. 275, č. 276, s. 31-34. ISSN 0022-2852.

Pracna, Petr ; Ceausu-Velcescu, A. ; Horneman, V. M. The ground and $v_6=1$ vibrational levels of HC₃₅Cl₃: The first high-resolution analysis of the v_6 fundamental band. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 2012, Roč. 113, č. 11, s. 1220-1225. ISSN 0022-4073.

Procházková, Dana ; Kurfiřtová, Lenka ; Pavlatová, Jana. Acylation of p-xylene over zeolites. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 78-84. ISSN 0920-5861.

Rajkumar, J. ; Schwederski, B. ; Fiedler, Jan ; Kaim, W. Facilitated reduction and oxidation of $\{[\text{Ru}(\text{NH}_3)_5]_4(\mu_4\text{-TCNX})\}_8^+$ by changing from TCNX = TCNQ to TCNQF4. *Polyhedron*, 2012, Roč. 44, č. 1, s. 174-178. ISSN 0277-5387.

Ramešová, Šárka ; Sokolová, Romana ; Degano, I. ; Bulíčková, Jana ; Žabka, Ján ; Gál, Miroslav. On the stability of the bioactive flavonoids quercetin and luteolin under oxygen-free conditions. *Analytical and Bioanalytical Chemistry*, 2012, Roč. 402, č. 2, s. 975-982. ISSN 1618-2642.

Roy, S. ; Sarkar, B. ; Imrich, H.-G. ; Fiedler, Jan ; Záliš, Stanislav ; Jimenez-Aparicio, R. ; Urbanos, F. A. ; Mobin, S. M. ; Lahiri, G. K. ; Kaim, W. Charged, but Found "Not Guilty": Innocence of the Suspect Bridging Ligands $[\text{RO}(\text{O})\text{CN}(\text{O})\text{OR}]^{(2-)} = \text{L}2^-$ in $[(\text{acac})_2\text{Ru}(\mu-\text{L})\text{Ru}(\text{acac})_2](\text{n})$, n = +,0,-,2-. *Inorganic Chemistry*, 2012, Roč. 51, č. 17, s. 9273-9281. ISSN 0020-1669.

Ruggeri, M. P. ; Grossale, A. ; Nova, I. ; Tronconi, E. ; Jirglová, Hana ; Sobalík, Zdeněk. FTIR in situ mechanistic study of the NH₃-NO/NO₂ "Fast SCR" reaction over a commercial Fe-ZSM-5 catalyst. *Catalysis Today*, 2012, Roč. 184, č. 1, s. 107-114. ISSN 0920-5861.

Samec, Zdeněk. Dynamic electrochemistry at the interface between two immiscible electrolytes. *Electrochimica acta*, 2012, Roč. 84, December, s. 21-28. ISSN 0013-4686.

Saniga, M. ; Levay, P. ; Pracna, Petr. Charting the Real Four-Qubit Pauli Group via Ovoids of a Hyperbolic Quadric of PG(7,2). *Journal of Physics A-Mathematical and Theoretical*, 2012, Roč. 45, JUL 27 2012, s. 295304. ISSN 1751-8113.

Saniga, M. ; Planat, M. ; Pracna, Petr ; Levay, P. 'Magic' Configurations of Three-Qubit Observables and Geometric Hyperplanes of the Smallest Split Cayley Hexagon. *Symmetry, Integrability and Geometry: Methods and Applications*, 2012, Roč. 8, č. 2012, 083. ISSN 1815-0659.

Shaffer, Christopher ; Schröder, Detlef ; Alcaraz, Ch. ; Žabka, Ján ; Zins, E. L. Reactions of Doubly Ionized Benzene with Nitrogen and Water: A Nitrogen-Mediated Entry into Superacid Chemistry. *ChemPhysChem*, 2012, Roč. 13, č. 11, s. 2688-2698. ISSN 1439-4235.

Shaffer, Christopher ; Schröder, Detlef ; Zins, E. L. ; Alcaraz, Ch. ; Žabka, Ján ; Roithová, J. Unimolecular dissociation of doubly ionized toluene and electron transfer between neutral toluene and its dication. *Chemical Physics Letters*, 2012, Roč. 534, 1 May, s. 8-12. ISSN 0009-2614.

Shamzy, M. V. ; Shvets, O. V. ; Opanasenko, V. ; Yaremov, P. S. ; Sarkisyan, L. G. ; Chlubná, Pavla ; Zukal, Arnošt ; Marthala, V. R. ; Hartmann, M. ; Čejka, Jiří. Synthesis of isomorphously substituted extra-large pore UTL zeolites. *Journal of Materials Chemistry*, 2012, Roč. 22, č. 31, s. 15793-15803. ISSN 0959-9428.

Shestivska, Violetta ; Španěl, Patrik ; Dryahina, Kseniya ; Sovová, Kristýna ; Smith, D. ; Musílek, M. ; Němec, A. Variability in the concentrations of volatile metabolites emitted by

genotypically different strains of *Pseudomonas aeruginosa*. *Journal of Applied Microbiology*, 2012, Roč. 113, č. 3, s. 701-713. ISSN 1364-5072.

Shinde, Tushar ; Žilková, Naděžda ; Hanková, V. ; Balcar, Hynek. Hoveyda-Grubbs type metathesis catalyst immobilized on mesoporous molecular sieves-The influence of pore size on the catalyst activity. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 123-129. ISSN 0920-5861.

Sikora, A. ; Woszczyna, M. ; Friedemann, M. ; Ahlers, F. J. ; Kalbáč, Martin. AFM diagnostics of graphene-based quantum Hall devices. *Micron*, 2012, Roč. 43, 2-3, s. 479-486. ISSN 0968-4328.

Smith, D. ; Sovová, Kristýna ; Španěl, Patrik. A selected ion flow tube study of the reactions of H₃O+, NO+ and O-2(+center dot) with seven isomers of hexanol in support of SIFT-MS. *International Journal of Mass Spectrometry*, 2012, Roč. 319, MAY 1 2012, s. 25-30. ISSN 1387-3806.

Sobalík, Zdeněk ; Tabor, Edyta ; Nováková, Jana ; Sathu, Naveen Kumar ; Závěta, K. Role of active oxygen and NOx species in N₂O decomposition over Fe-ferrierite. *Journal of Catalysis*, 2012, Roč. 289, MAY 2012, s. 164-170. ISSN 0021-9517.

Sokolová, Romana ; Gál, Miroslav ; Valášek, M. New Proton Donors in Electrochemical Mechanistic Studies in Non-Aqueous Solution Dimethylsulfoxide. Chlorinated Hydroxybenzonitriles. *Journal of Electroanalytical Chemistry*, 2012, Roč. 685, OCT 1 2012, s. 33-36. ISSN 1572-6657.

Sokolová, Romana ; Ramešová, Šárka ; Degano, I. ; Hromadová, Magdaléna ; Gál, Miroslav ; Žabka, Ján. The oxidation of natural flavonoid quercetin. *Chemical Communications*, 2012, Roč. 48, č. 28, s. 3433-3435. ISSN 1359-7345.

Sovová, Kristýna ; Shestivska, Violetta ; Španěl, Patrik. Real-Time Quantification of Traces of Biogenic Volatile Selenium Compounds in Humid Air by Selected Ion Flow Tube Mass Spectrometry. *Analytical Chemistry*, 2012, Roč. 84, č. 11, s. 4979-4983. ISSN 0003-2700.

Strachotová, Dita ; Holoubek, A. ; Kučerová, Helena ; Benda, Aleš ; Humpolíčková, Jana ; Váchová, Libuše ; Palková, Z. Ato protein interactions in yeast plasma membrane revealed by fluorescence lifetime imaging (FLIM). *Biochimica Et Biophysica Acta-Biomembranes*, 2012, Roč. 1818, č. 9, s. 2126-2134. ISSN 0005-2736.

Szeifert, J. M. ; Fattakhova-Rohlfing, D. ; Rathouský, Jiří ; Bein, T. Multilayered High Surface Area "Brick and Mortar" Mesoporous Titania Films as Efficient Anodes in Dye-Sensitized Solar Cells. *Chemistry of Materials*, 2012, Roč. 24, č. 4, s. 659-663. ISSN 0897-4756.

Šachl, Radek ; Johansson, L. B. A. ; Hof, Martin. Förster Resonance Energy Transfer (FRET) between Heterogeneously Distributed Probes: Application to Lipid Nanodomains and Pores. *International Journal of Molecular Sciences*, 2012, Roč. 13, č. 12, s. 16141-16156. ISSN 1422-0067.

Šelešovská, R. ; Bandžuchová, L. ; Navrátil, Tomáš ; Chýlková, J. Voltammetric determination of leucovorin using silver solid amalgam electrode. *Electrochimica acta*, 2012, Roč. 60, JAN 15 2012, s. 375-383. ISSN 0013-4686.

Šimsa, Daniel ; Demel, Ondřej ; Bhaskaran-Nair, Kiran ; Hubač, I. ; Mach, P. ; Pittner, Jiří. Multireference coupled cluster study of the oxyallyl diradical. *Chemical Physics*, 2012, Roč. 401, JUN 5 2012, s. 203-207. ISSN 0301-0104.

Štefl, Martin ; Šachl, Radek ; Humpolíčková, Jana ; Cebecauer, Marek ; Macháň, Radek ; Kolářová, Marie ; Johansson, L. B. A. ; Hof, Martin. Dynamics and Size of Cross-Linking-Induced Lipid Nanodomains in Model Membranes. *Biophysical Journal*, 2012, Roč. 102, č. 9, s. 2104-2113. ISSN 0006-3495.

Tan, B. K. ; Davies, S. J. ; Španěl, Patrik ; Smith, D. Injection of deuterated water into the pulmonary/alveolar circulation; measurement of HDO in exhaled breath and implications to breath analysis. *Journal of Breath Research*, 2012, Roč. 6, č. 3, 036005. ISSN 1752-7155.

Teplý, Filip ; Čížková, Martina ; Slavíček, P. ; Kolivoška, Viliam ; Tarábek, Ján ; Hromadová, Magdaléna ; Pospíšil, Lubomír. Electron Transfer Triggers Fast Dimer/Monomer Switching of Pyridinium and Quinolinium Cations. *Journal of Physical Chemistry C*, 2012, Roč. 116, č. 5, s. 3779-3786. ISSN 1932-7447.

Trojánek, Antonín ; Langmaier, Jan ; Záliš, Stanislav ; Samec, Zdeněk. Competitive inhibition of a metal-free porphyrin oxygen-reduction catalyst by water. *Chemical Communications*, 2012, Roč. 48, č. 34, s. 4094-4096. ISSN 1359-7345.

Trojánek, Antonín ; Langmaier, Jan ; Samec, Zdeněk. Thermodynamic driving force effects in the oxygen reduction catalyzed by a metal-free porphyrin. *Electrochimica acta*, 2012, Roč. 82, SI, s. 457-462. ISSN 0013-4686.

Uras-Aytemiz, N. ; Cwiklik, Lukasz ; Devlin, J. P. Tracking all-vapor instant gas-hydrate formation and guest molecule populations: A possible probe for molecules trapped in water nanodroplets. *Journal of Chemical Physics*, 2012, Roč. 137, č. 20, s. 204501. ISSN 0021-9606.

Varga, V. ; Gyepes, R. ; Pinkas, Jiří ; Horáček, Michal ; Kubišta, Jiří ; Mach, Karel. Ion pairs from redox reaction of decamethylchromocene with cyclopentadienyltitanium trichlorides. *Inorganic Chemistry Communications*, 2012, Roč. 19, MAY 2012, s. 61-65. ISSN 1387-7003.

Varga, V. ; Horáček, Michal ; Bastl, Zdeněk ; Merna, J. ; Císařová, I. ; Sýkora, Jan ; Pinkas, Jiří. Zirconocene silanolate complexes and their heterogeneous siliceous analogues as catalysts for phenylsilane dehydropolymerization. *Catalysis Today*, 2012, Roč. 179, č. 1, s. 130-139. ISSN 0920-5861.

Vazdar, Mario ; Jurkiewicz, Piotr ; Hof, Martin ; Jungwirth, Pavel ; Cwiklik, Lukasz. Behavior of 4-Hydroxynonenal in Phospholipid Membranes. *Journal of Physical Chemistry B*, 2012, Roč. 116, č. 22, s. 6411-6415. ISSN 1520-6106.

Veis, Libor ; Višňák, Jakub ; Fleig, T. ; Knecht, S. ; Saue, T. ; Visscher, L. ; Pittner, Jiří. Relativistic quantum chemistry on quantum computers. *Physical Review. A*, 2012, Roč. 85, č. 3, 030304. ISSN 1050-2947.

Verdanová, M. ; Brož, A. ; Kalbáč, Martin ; Kalbáčová, M. Influence of oxygen and hydrogen treated graphene on cell adhesion in the presence or absence of fetal bovine serum. *Physica Status Solidi B-Basic Solid State Physics*, 2012, Roč. 249, č. 12, s. 2503-2506. ISSN 0370-1972.

Verdanová, M. ; Brož, A. ; Kalbáč, Martin ; Kalbáčová, M. Influence of oxygen and hydrogen treated graphene on cell adhesion in the presence or absence of fetal bovine serum. *Physica Status Solidi B-Basic Solid State Physics*, 2012, Roč. 249, č. 12, s. 2503-2506. ISSN 0370-1972.

Wahab, Abdul ; Stepp, Brian R. ; Douvris, C. ; Valášek, Michal ; Štursa, Jan ; Klíma, Jiří ; Piqueras, M. C. ; Crespo, R. ; Ludvík, Jiří ; Michl, Josef. Measured and Calculated Oxidation Potentials of 1-X-12-Y-CB11Me10- Anions. *Inorganic Chemistry*, 2012, Roč. 51, č. 9, s. 5128-5137. ISSN 0020-1669.

Wang, J. ; Sklenák, Štěpán ; Liu, A. ; Felczak, K. ; Wu, Y. ; Li, Y. ; Yan, H. Role of Glutamate 64 in the Activation of the Prodrug 5-Fluorocytosine by Yeast Cytosine Deaminase. *Biochemistry*, 2012, Roč. 51, č. 1, s. 475-486. ISSN 0006-2960.

Wild, J. ; Kudrna, P. ; Tichý, M. ; Nevrly, V. ; Střížík, M. ; Bitala, P. ; Filipi, B. ; Zelinger, Zdeněk. Electron Temperature Measurement in a Premixed Flat Flame Using the Double Probe Method. *Contributions to Plasma Physics*, 2012, Roč. 52, č. 8, s. 692-698. ISSN 0863-1042.

Yosypchuk, O. ; Barek, J. ; Yosypchuk, Bogdan. Tubular Detector of Silver Solid Amalgam for Electrochemical Measurements in Flow Systems. *Electroanalysis*, 2012, Roč. 24, č. 12, s. 2230-2234. ISSN 1040-0397.

Zakharov, S. ; Navrátil, Tomáš ; Pelcová, D. Analysis of Medication Errors of Health Care Providers on the Basis of Data from the Czech Toxicological Information Centre over an 11-Year Period (2000-2010). *Basic & Clinical Pharmacology & Toxicology*, 2012, Roč. 110, č. 5, s. 427-432. ISSN 1742-7835.

Zimpl, M. ; Skopalová, J. ; Jirovský, D. ; Barták, P. ; Navrátil, Tomáš ; Sedoníková, J. ; Kotouček, M. Electrochemical Behavior of Quinoxalin-2-one Derivatives at Mercury Electrodes and Its Analytical Use. *TheScientificWorldJOURNAL*, 2012, Roč. 2012, č. 2012, s. 409378. ISSN 1537-744X.
<http://www.tswj.com/2012/409378/>

Žabka, Ján ; Romanzin, C. ; Alcaraz, Ch. ; Polášek, Miroslav. Anion chemistry on Titan: A possible route to large N-bearing hydrocarbons. *Icarus*, 2012, Roč. 219, č. 1, s. 161-167. ISSN 0019-1035.

Monographs and contributions in Monographs (1, 7)

Čársky, Petr (ed.) ; Čurík, Roman (ed.). *Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces*. 1. Boca Raton : CRC Press, Taylor & Francis Group, 2012. 286 s. ISBN 978-1-4398-3910-2. 1.

Cebecauer, Marek ; Humpolíčková, Jana ; Rossy, J. Advanced Imaging of Cellular Signaling Events. In *Methods in Enzymology. Imaging and Spectroscopic Analysis of Living CellsLive Cell Imaging of Cellular Elements and Functions*. Vol. 505.. Amsterdam : Elsevier, 2012. S. 273-289. ISBN 978-0-12-388448-0.

Čársky, Petr ; Čurík, Roman. Vibrational excitations of polyatomic molecules. In Čársky, Petr; Čurík, Roman (ed.). *Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces* 1.. Boca Raton : CRC Press, Taylor & Francis Group, 2012. S. 263-282. ISBN 978-1-4398-3910-2.

Čurík, Roman ; Horáček, J. Introduction to numerical methods. In Čársky, Petr; Čurík, Roman (ed.). *Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces* 1.. Boca Raton : CRC Press, Taylor & Francis Group, 2012. S. 9-43. ISBN 978-1-4398-3910-2.

Dolejšek, Zdeněk. Přesmyky iontů a má spolupráce s Vladimírem Hanušem v Ústavu fyzikální chemie ČSAV (1957-1964). In *Počátky a historie Československé hmotnostní spektrometrie*. Praha : Česká společnost pro hmotnostní spektrometrii, 2012. S. 43-49. ISBN 978-80-905045-2-3.

Przybylo, M. ; Procek, J. ; Kaczynski, M. ; Borowik, T. ; Hof, Martin ; Langner, M. A Multi Time-Scale Approach of the Lipid Bilayer Dynamics. In Iglič, A. (ed.). *ADVANCES IN PLANAR LIPID BILAYERS AND LIPOSOMES*. San Diego : Elsevier, 2012. S. 105-137. ISBN 978-0-12-396533-2.

Rathouský, Jiří ; Kalousek, Vít ; Žouželka, Radek. Nanomaterials and nanotechnologies for the conservation of the materials of cultural heritage. In *Nanotechnology 2012: Advanced Materials, CNTs, Particles, Films and Composites* Vol. 1. 1.. Danville : Nano Science and Technology Institute, 2012. S. 417-420. ISBN 978-1-4665-6274-5.

Schauer, Jan ; Kočířík, Milan. Membránové materiály. In Palatý, Z. (ed.). *Membránové procesy*. Praha : Vysoká škola chemicko-technologická v Praze, 2012. S. 67-107. ISBN 978-80-7080-808-5.

 http://vydavatelstvi.vscht.cz/katalog/uid_isbn-978-80-7080-808-5/anotace/