

## Научни публикации на проф. дхн Георги Николов Вайсилов

(до май 2024 г.)

Научни статии и обзори в списания с импакт фактор: 150

Глави в книги: 5

Научни статии и обзори в други списания и сборници от конференции: 7

Общо: 162

### Научни статии и обзори в списания с импакт фактор

150. Stoyan P. Gramatikov, Petko St. Petkov, Zhendong Wang, Weimin Yang, Georgi N. Vayssilov

„Variation of the Orientations of Organic Structure-Directing Agents inside the Channels of SCM-14 and SCM-15 Germanosilicates Obtained by Ab Initio Molecular Dynamic Simulations“  
Nanomaterials 14, 159 (2024).

149. Mohammad Fahda, Jawad Fayek, Eddy Dib, Hugo Cruchade, Nathan Pichot, Nourrdine Chaouati, Ludovic Pinard, Petko St. Petkov, Georgi N. Vayssilov, Alvaro Mayoral, Bernhard Witulski, Louwanda Lakiss, and Valentin Valtchev

“Investigating the Physicochemical Properties of an Extra-large Pore Aluminosilicate ZEO-1”  
Chemistry of Materials 2024, <https://doi.org/10.1021/acs.chemmater.4c00186>

148. Kristina K. Chakarova, Videlina R. Zdravkova, Bayan S. Karapenchev, Diana D. Nihtianova, Elena Z. Ivanova, Hristiyan A. Aleksandrov, Iskra Z. Koleva, Dimitar A. Panayotov, Mihail Y. Mihaylov, Georgi N. Vayssilov, Konstantin I. Hadjiivanov

„Evolution of Ce<sup>4+</sup> Lewis acidity during dehydroxylation of ceria nanoparticles with different morphology: An integrated FTIR, DFT and HRTEM study“  
Journal of Catalysis 433, 115463 (2024).

147. Stoyan P. Gramatikov, Petko St. Petkov, Zhendong Wang, Weimin Yang, Georgi N. Vayssilov

„The interaction of the structure-directing agent with the zeolite framework determines germanium distribution in SCM-15 germanosilicate“  
Frontiers of Chemical Science and Engineering 18, 58 (2024).

146. Nikola Drenchev, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Borislav Shivachev, Konstantin Hadjiivanov

„Why does CaX zeolite have such a high CO<sub>2</sub> capture capacity and how is it affected by water?“  
Separation and Purification Technology, 349, 127662 (2024).

145. Edwin B Clatworthy, Simona Moldovan, Kalthoum Nakouri, Stoyan P. Gramatikov, Francesco Dalena, Marco Daturi, Petko St. Petkov, Georgi N. Vayssilov, Svetlana Mintova

“Visualizing the Flexibility of RHO Nanozeolite: Experiment and Modeling”  
Journal of the American Chemical Society, 145, 15313-15323 (2023).

144. Peng Peng, Simona Moldovan, Aurélie Vicente, Valérie Ruaux, Maxime Debost, Han Hu, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Zi-Feng Yan, Svetlana Mintova  
“Synthesis of nanosized MFI zeolites using Cu-containing complexes”  
Microporous and Mesoporous Materials, 357, 112625 (2023).
143. Eddy Dib, Svetlana Mintova, Georgi N. Vayssilov, Hristiyan A. Aleksandrov, Marina Carravetta  
“Chemical Shift Anisotropy: A Promising Parameter To Distinguish the  $^{29}\text{Si}$  NMR Peaks in Zeolites.”  
Journal of Physical Chemistry C, 127, 10792–10796 (2023).
142. Iskra Z. Koleva, Hristiyan A. Aleksandrov, and Georgi N. Vayssilov  
“Comparison of the Reactivity of Platinum Cations and Clusters Supported on Ceria or Alumina in Carbon Monoxide Oxidation”  
ACS Catalysis, 13, 5358–5374 (2023).
141. Konstantin Khivantsev, Nicholas R. Jaegers, Hristiyan A. Aleksandrov, Inhak Song, Xavier Isidro Pereira-Hernandez, Mark H. Engelhard, Jinshu Tian, Linxiao Chen, Debora Motta Meira, Libor Kovarik, Georgi N. Vayssilov, Yong Wang, János Szanyi  
“Single Ru (II) Ions on Ceria as a Highly Active Catalyst for Abatement of NO”  
Journal of the American Chemical Society 145, 9, 5029–5040 (2023).
140. Dong Gun Oh, Hristiyan A. Aleksandrov, Haneul Kim, Iskra Z. Koleva, Konstantin Khivantsev, Georgi N. Vayssilov, Ja Hun Kwak  
“Understanding of Active Sites and Interconversion of Pd and PdO during  $\text{CH}_4$  Oxidation”  
Molecules 28 (4), 1957 (2023).
139. Nikola L. Drenchev, Elena Z. Ivanova, Mihail Y. Mihaylov, Hristiyan A. Aleksandrov, Georgi N Vayssilov, Konstantin I Hadjiivanov  
“One  $\text{Ca}^{2+}$  Site in CaNaY Zeolite Can Attach Three  $\text{CO}_2$  Molecules”  
Journal of Physical Chemistry Letters 14 (6), 1564-1569 (2023).
138. Matthias Nuber, Lukas V. Spanier, Sebastian Roth, Georgi N. Vayssilov, Reinhard Kienberger, Peter Müller-Buschbaum, Hristo Iglev  
“Picosecond Charge-Transfer-State Dynamics in Wide Band Gap Polymer–Non-Fullerene Small-Molecule Blend Films Investigated via Transient Infrared Spectroscopy”  
Journal of Physical Chemistry Letters 13 (44), 10418-10423 (2022)
137. Georgi N. Vayssilov, Hristiyan A. Aleksandrov, Eddy Dib, Izabel Medeiros Costa, Nikolai Nesterenko, Svetlana Mintova  
“Superacidity and spectral signatures of hydroxyl groups in zeolites”  
Microporous and Mesoporous Materials, 343, 112144 (2022)
136. Konstantin Khivantsev, Ja-Hun Kwak, Nicholas R. Jaegers, Iskra Z. Koleva, Georgi N. Vayssilov, Mirosław A. Derewinski, Yong Wang, Hristiyan A. Aleksandrov, Janos Szanyi  
“Identification of the mechanism of NO reduction with ammonia (SCR) on zeolite catalysts”  
Chemical Science, 2022, 13, 10383-10394
135. Dong Gun Oh, Hristiyan A. Aleksandrov, Haneul Kim, Iskra Z. Koleva, Konstantin Khivantsev, Georgi N. Vayssilov, Ja Hun Kwak

"Key Role of a-Top CO on Terrace Sites of Metallic Pd Clusters for CO Oxidation"  
Chemistry–A European Journal, 28, e202200684 (2022)

134. Oriol Piqué, Iskra Z. Koleva, Albert Bruix, Francesc Vines, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Francesc Illas

"Charting the Atomic C Interaction with Transition Metal Surfaces"

ACS Catalysis, 12, 9256-9269 (2022)

133. Stefan K. Kolev, Petko St. Petkov, Teodor I. Milenov, Georgi N. Vayssilov

"Sodium and Magnesium Ion Location at the Backbone and at the Nucleobase of RNA: Ab Initio Molecular Dynamics in Water Solution"

ACS omega, 7, 23234-23244 (2022)

132. Stoyan P. Gramatikov, Petko St. Petkov, Georgi N. Vayssilov

"The relative stability of SCM-14 germanosilicate with different distributions of germanium ions in the absence and presence of structure-directing agents"

Inorganic Chemistry Frontiers, 9, 3747-3757 (2022)

131. Naonobu Katada, Kana Yamamoto, Moeri Fukui, Kai Asanuma, Satoshi Inagaki, Kazuki Nakajima, Satoshi Suganuma, Etsushi Tsuji, Ana Palcic, Valentin Valtchev, Petko St. Petkov, Kristina Simeonova, Georgi N. Vayssilov, Yoshihiro Kubota

"Acidic property of YNU-5 zeolite influenced by its unique micropore system"

Microporous and Mesoporous Materials, 330, 111592 (2022).

130. Izabel C Medeiros-Costa, Eddy Dib, Florent Dubray, Simona Moldovan, Jean-Pierre Gilson, Jean-Pierre Dath, Nikolai Nesterenko, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Svetlana Mintova

"Unraveling the Effect of Silanol Defects on the Insertion of Single-Site Mo in the MFI Zeolite Framework"

Inorganic Chemistry 61, 1418–1425 (2022).

129. Zhengxing Qin, Zhenchao You, Krassimir N. Bozhilov, Stefan K. Kolev, Wei Yang, Yanfeng Shen, Xin Jin, Jean-Pierre Gilson, Svetlana Mintova, Georgi N. Vayssilov, Valentin Valtchev

"Dissolution Behavior and Varied Mesoporosity of Zeolites by NH<sub>4</sub>F Etching"

Chemistry–A European Journal 28, e202104339 (2022).

128. Louwanda Lakiss, Cassandre Kouvatas, Jean-Pierre Gilson, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Nikolai Nesterenko, Svetlana Mintova, Valentin Valtchev

"Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism"

Angewandte Chemie International Edition, 60, 26702-26709 (2021).

127. Petko St. Petkov, Kristina Simeonova, Iskra Z. Koleva, Hristiyan A. Aleksandrov, Yoshihiro Kubota, Satoshi Inagaki, Valentin Valtchev, Georgi N. Vayssilov

"Defect Formation, T-Atom Substitution and Adsorption of Guest Molecules in MSE-Type Zeolite Framework—DFT Modeling"

Molecules, 26, 7296 (13 pp.) (2021)

126. Konstantin Khivantsev, Nicholas R. Jaegers, Hristiyan A. Aleksandrov, Libor Kovarik, Mirosław A Derewinski, Yong Wang, Georgi N. Vayssilov, Janos Szanyi  
“Biomimetic CO oxidation below– 100° C by a nitrate-containing metal-free microporous system”  
Nature Communications, 12, 6033 (2021).
125. Eddy Dib, Izabel Medeiros Costa, Georgi N. Vayssilov, Hristiyan A. Aleksandrov, Svetlana Mintova  
“Complex H-bonded silanol network in zeolites revealed by IR and NMR spectroscopy combined with DFT calculations”  
Journal of Materials Chemistry A 9 (48), 27347-27352 (2021).
124. Konstantin Khivantsev, Artem Vityuk, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Oleg S. Alexeev, and Michael D. Amiridis  
“Catalytic conversion of ethylene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route”  
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123. M. Y. Mihaylov, V. R. Zdravkova, E. Z. Ivanova, H. A. Aleksandrov, P. St. Petkov, G. N. Vayssilov, K. I. Hadjiivanov  
“Infrared spectra of surface nitrates: Revision of the current opinions based on the case study of ceria”  
Journal of Catalysis 394, 245-258 (2021).
122. Margarita Popova, Neli Koseva, Ivalina Trendafilova, Hristina Lazarova, Violeta Mitova, Judith Mihály, Denitsa Momekova, Spiro Konstantinov, Iskra Z. Koleva, Petko St. Petkov, Georgi N. Vayssilov, Hristiyan A. Aleksandrov, Agnes Szegedi  
“Design of PEG-modified magnetic nanoporous silica based miltefosine delivery system: Experimental and theoretical approaches”  
Microporous and Mesoporous Materials 310, 110664 (2021).
121. I. Z. Koleva, H. A. Aleksandrov, K. M. Neyman, G. N. Vayssilov  
“Preferential location of zirconium dopants in cerium dioxide nanoparticles and the effects of doping on their reducibility: a DFT study”  
Physical Chemistry Chemical Physics 22, 26568-26582 (2020).
120. Margarita Popova, Neli Koseva, Ivalina Trendafilova, Hristina Lazarova, Violeta Mitova, Judith Mihály, Denitsa Momekova, Georgi Momekov, Iskra Z. Koleva, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Ágnes Szegedi  
“Tamoxifen Delivery System Based on PEGylated Magnetic MCM-41 Silica”  
Molecules 25, 5129 (2020).
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“Revisiting ceria-NO<sub>x</sub> interaction: FTIR studies”  
Catalysis Today 357, 613-620 (2020).
118. Iskra Z. Koleva, Hristiyan A. Aleksandrov, Georgi N. Vayssilov  
“Influence of the adsorption of CO on the electronic structure of platinum clusters and nanowires

deposited on CeO<sub>2</sub> (111) and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (001) surfaces”  
Catalysis Today 357, 442-452 (2020).

117. Konstantin Khivantsev, Nicholas R Jaegers, Iskra Z Koleva, Hristiyan A Aleksandrov, Libor Kovarik, Mark Engelhard, Feng Gao, Yong Wang, Georgi N Vayssilov, Janos Szanyi  
“Stabilization of Super Electrophilic Pd<sup>+2</sup> Cations in Small-Pore SSZ-13 Zeolite”  
Journal of Physical Chemistry C 124, 309-321 (2020).

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“Paraquat adsorption on NaY zeolite at various Si/Al ratios: a combined experimental and computational study”  
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115. Margarita Popova, Rositsa Mihaylova, Georgi Momekov, Denitsa Momekova, Hristina Lazarova, Ivalina Trendafilova, Violeta Mitova, Neli Koseva, Judith Mihályi, Pavletta Shestakova, Petko St. Petkov, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Spiro Konstantinov, Ágnes Szegedi  
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“Characterization and temperature evolution of iron-containing species in HZSM-5 zeolite prepared from different iron sources”  
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“Hydrophobic Tungsten-Containing MFI-Type Zeolite Films for Exhaust Gas Detection”  
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“Subsurface carbon: a general feature of noble metals”  
Angewandte Chemie International Edition 58, 1744-1748 (2019).

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Journal of Drug Delivery Science and Technology 49, 700-712 (2019).

110. Krassimira Yoncheva, Maria Merino, Aslihan Shenol, Nikolay T. Daskalov, Petko St. Petkov, Georgi N. Vayssilov, Maria J. Garrido  
“Optimization and in-vitro/in-vivo evaluation of doxorubicin-loaded chitosan-alginate nanoparticles using a melanoma mouse model”  
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109. Artem Vityuk, Konstantin Khivantsev, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Oleg S. Alexeev, Michael D. Amiridis,  
“Room Temperature Ethene Hydrogenation Activity of Transition-Metal-Free HY Zeolites”  
ACS Catalysis 9, 839–847 (2019).
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Angewandte Chemie Int. Ed. 57, 16672-16677 (2018).
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Microporous and Mesoporous Materials 270, 40-47 (2018).
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“Structure and reducibility of doped by yttrium cerium dioxide nanoparticles and (111) surface”  
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“Interaction of Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup> and Ca<sup>2+</sup> Counter Cations with RNA”  
Metallomics 10, 659-678 (2018). (*on the Journal cover*)
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“Computational elucidation of the reaction mechanism for synthesis of pyrrolidinedione derivatives via Nef-type rearrangement–cyclization reaction.”  
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 “Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling”  
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