

# Kirill A Lomachenko

## List of Publications by Citations

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88

papers

3,727

citations

32

h-index

60

g-index

91

ext. papers

4,405

ext. citations

5.1

avg, IF

5.36

L-index

| #  | Paper   | IF   | Citations |
|----|---|------|-----------|
| 88 | A Consistent Reaction Scheme for the Selective Catalytic Reduction of Nitrogen Oxides with Ammonia. <i>ACS Catalysis</i> , <b>2015</b> , 5, 2832-2845   | 13.1 | 319       |
| 87 | Revisiting the nature of Cu sites in the activated Cu-SSZ-13 catalyst for SCR reaction. <i>Chemical Science</i> , <b>2015</b> , 6, 548-563  | 9.4  | 265       |
| 86 | Cerium-based metal organic frameworks with UiO-66 architecture: synthesis, properties and redox catalytic activity. <i>Chemical Communications</i> , <b>2015</b> , 51, 12578-81   | 5.8  | 249       |
| 85 | Interaction of NH <sub>3</sub> with Cu-SSZ-13 Catalyst: A Complementary FTIR, XANES, and XES Study. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 1552-9  | 6.4  | 209       |
| 84 | Methane to Methanol: Structure-Activity Relationships for Cu-CHA. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 14961-14975  | 16.4 | 202       |
| 83 | Metal-organic frameworks: structure, properties, methods of synthesis and characterization. <i>Russian Chemical Reviews</i> , <b>2016</b> , 85, 280-307   | 6.8  | 198       |
| 82 | The Cu-CHA deNO <sub>x</sub> Catalyst in Action: Temperature-Dependent NH <sub>3</sub> -Assisted Selective Catalytic Reduction Monitored by Operando XAS and XES. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 12025-8                      | 16.4 | 197       |
| 81 | Optimized Finite Difference Method for the Full-Potential XANES Simulations: Application to Molecular Adsorption Geometries in MOFs and Metal-Ligand Intersystem Crossing Transients. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 4512-21 | 6.4  | 137       |
| 80 | Composition-driven Cu-speciation and reducibility in Cu-CHA zeolite catalysts: a multivariate XAS/FTIR approach to complexity. <i>Chemical Science</i> , <b>2017</b> , 8, 6836-6851   | 9.4  | 129       |
| 79 | The Nuclearity of the Active Site for Methane to Methanol Conversion in Cu-Mordenite: A Quantitative Assessment. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 15270-15278   | 16.4 | 123       |
| 78 | Probing Reactive Platinum Sites in UiO-67 Zirconium Metal-Organic Frameworks. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 1042-1056   | 9.6  | 95        |
| 77 | Reversible Capture and Release of Cl and Br with a Redox-Active Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 5992-5997   | 16.4 | 82        |
| 76 | In situ formation of hydrides and carbides in palladium catalyst: When XANES is better than EXAFS and XRD. <i>Catalysis Today</i> , <b>2017</b> , 283, 119-126  | 5.3  | 81        |
| 75 | High Zn/Al ratios enhance dehydrogenation vs hydrogen transfer reactions of Zn-ZSM-5 catalytic systems in methanol conversion to aromatics. <i>Journal of Catalysis</i> , <b>2018</b> , 362, 146-163  | 7.3  | 78        |
| 74 | Temperature- and Pressure-Dependent Hydrogen Concentration in Supported PdH <sub>x</sub> Nanoparticles by Pd K-Edge X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 10416-10423  | 3.8  | 73        |
| 73 | Unravelling the Redox-catalytic Behavior of Ce Metal-Organic Frameworks by X-ray Absorption Spectroscopy. <i>ChemPhysChem</i> , <b>2018</b> , 19, 373-378   | 3.2  | 69        |
| 72 | Synthesis of M-UiO-66 (M = Zr, Ce or Hf) employing 2,5-pyridinedicarboxylic acid as a linker: defect chemistry, framework hydrophilisation and sorption properties. <i>Dalton Transactions</i> , <b>2018</b> , 47, 1062-1070  | 4.3  | 65        |

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|----|--|------|----|
| 71 | Core-shell Structure of Palladium Hydride Nanoparticles Revealed by Combined X-ray Absorption Spectroscopy and X-ray Diffraction. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 18202-18213  | 3.8  | 57 |
| 70 | A Titanium(IV)-Based Metal-Organic Framework Featuring Defect-Rich Ti-O Sheets as an Oxidative Desulfurization Catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 9160-9165  | 16.4 | 53 |
| 69 | Structure and Reactivity of Oxygen-Bridged Diamino Dicopper(II) Complexes in Cu-Ion-Exchanged Chabazite Catalyst for NH <sub>3</sub> -Mediated Selective Catalytic Reduction. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 15884-15896 | 16.4 | 51 |
| 68 | Palladium Carbide and Hydride Formation in the Bulk and at the Surface of Palladium Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 12029-12037   | 3.8  | 45 |
| 67 | Quantitative structural determination of active sites from in situ and operando XANES spectra: From standard ab initio simulations to chemometric and machine learning approaches. <i>Catalysis Today</i> , <b>2019</b> , 336, 3-21                            | 5.3  | 44 |
| 66 | Exact Stoichiometry of Ce Zr Cornerstones in Mixed-Metal UiO-66 Metal-Organic Frameworks Revealed by Extended X-ray Absorption Fine Structure Spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 17379-17383                   | 16.4 | 44 |
| 65 | Evolution of active sites during selective oxidation of methane to methanol over Cu-CHA and Cu-MOR zeolites as monitored by operando XAS. <i>Catalysis Today</i> , <b>2019</b> , 333, 17-27  | 5.3  | 43 |
| 64 | Exploring structure and reactivity of Cu sites in functionalized UiO-67 MOFs. <i>Catalysis Today</i> , <b>2017</b> , 283, 89-103   | 5.3  | 42 |
| 63 | Time-resolved operando studies of carbon supported Pd nanoparticles under hydrogenation reactions by X-ray diffraction and absorption. <i>Faraday Discussions</i> , <b>2018</b> , 208, 187-205   | 3.6  | 42 |
| 62 | Modulator Effect in UiO-66-NDC (1,4-Naphthalenedicarboxylic Acid) Synthesis and Comparison with UiO-67-NDC Isorecticular Metal-Organic Frameworks. <i>Crystal Growth and Design</i> , <b>2017</b> , 17, 5422-5431  | 3.5  | 42 |
| 61 | Solvent-Driven Gate Opening in MOF-76-Ce: Effect on CO <sub>2</sub> Adsorption. <i>ChemSusChem</i> , <b>2016</b> , 9, 713-9  | 8.3  | 42 |
| 60 | Nitrate/nitrite equilibrium in the reaction of NO with a Cu-CHA catalyst for NH <sub>3</sub> -SCR. <i>Catalysis Science and Technology</i> , <b>2016</b> , 6, 8314-8324  | 5.5  | 39 |
| 59 | Operando study of palladium nanoparticles inside UiO-67 MOF for catalytic hydrogenation of hydrocarbons. <i>Faraday Discussions</i> , <b>2018</b> , 208, 287-306   | 3.6  | 37 |
| 58 | Temperature-dependent dynamics of NH <sub>3</sub> -derived Cu species in the Cu-CHA SCR catalyst. <i>Reaction Chemistry and Engineering</i> , <b>2019</b> , 4, 1067-1080   | 4.9  | 33 |
| 57 | Identifying Cu-oxo species in Cu-zeolites by XAS: A theoretical survey by DFT-assisted XANES simulation and EXAFS wavelet transform. <i>Catalysis Today</i> , <b>2020</b> , 345, 125-135   | 5.3  | 33 |
| 56 | High energy resolution core-level X-ray spectroscopy for electronic and structural characterization of osmium compounds. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 16152-9  | 3.6  | 32 |
| 55 | Tuning Pt and Cu sites population inside functionalized UiO-67 MOF by controlling activation conditions. <i>Faraday Discussions</i> , <b>2017</b> , 201, 265-286   | 3.6  | 27 |
| 54 | A Titanium(IV)-Based Metal-Organic Framework Featuring Defect-Rich Ti-O Sheets as an Oxidative Desulfurization Catalyst. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 9258-9263   | 3.6  | 25 |

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|----|---|------|----|
| 53 | The duality of UiO-67-Pt MOFs: connecting treatment conditions and encapsulated Pt species by operando XAS. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 27489-27507                          | 3.6  | 25 |
| 52 | Co-Ligand Dependent Formation and Phase Transformation of Four Porphyrin-Based Cerium Metal-Organic Frameworks. <i>Crystal Growth and Design</i> , <b>2017</b> , 17, 3462-3474                                  | 3.5  | 23 |
| 51 | XAS and XES Techniques Shed Light on the Dark Side of Ziegler-Natta Catalysts: Active-Site Generation. <i>ChemCatChem</i> , <b>2015</b> , 7, 1432-1437  | 5.2  | 23 |
| 50 | EXAFS wavelet transform analysis of Cu-MOR zeolites for the direct methane to methanol conversion. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 18950-18963                                   | 3.6  | 23 |
| 49 | Evidence of Mixed-Ligand Complexes in CuCHA by Reaction of Cu Nitrates with NO/NH <sub>3</sub> at Low Temperature. <i>ChemCatChem</i> , <b>2019</b> , 11, 3828-3838   | 5.2  | 22 |
| 48 | Hydride phase formation in carbon supported palladium hydride nanoparticles by in situ EXAFS and XRD. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012032                                  | 0.3  | 21 |
| 47 | Finite difference method accelerated with sparse solvers for structural analysis of the metal-organic complexes. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012004                       | 0.3  | 19 |
| 46 | The impact of reaction conditions and material composition on the stepwise methane to methanol conversion over Cu-MOR: An operando XAS study. <i>Catalysis Today</i> , <b>2019</b> , 336, 99-108                | 5.3  | 19 |
| 45 | Disclosing the Properties of a New Ce(III)-Based MOF: Ce <sub>2</sub> (NDC) <sub>3</sub> (DMF) <sub>2</sub> . <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 787-796                                      | 3.5  | 18 |
| 44 | Dynamics of Reactive Species and Reactant-Induced Reconstruction of Pt Clusters in Pt/Al <sub>2</sub> O <sub>3</sub> Catalysts. <i>ACS Catalysis</i> , <b>2019</b> , 9, 7124-7136                               | 13.1 | 15 |
| 43 | Evolution of Pt and Pd species in functionalized UiO-67 metal-organic frameworks. <i>Catalysis Today</i> , <b>2019</b> , 336, 33-39   | 5.3  | 13 |
| 42 | Understanding and Optimizing the Performance of Cu-FER for The Direct CH <sub>4</sub> to CH <sub>3</sub> OH Conversion. <i>ChemCatChem</i> , <b>2019</b> , 11, 621-627  | 5.2  | 13 |
| 41 | Finding the active species: The conversion of methanol to aromatics over Zn-ZSM-5/alumina shaped catalysts. <i>Journal of Catalysis</i> , <b>2021</b> , 394, 416-428  | 7.3  | 13 |
| 40 | ? Divergent coordination behavior of early-transition metals towards MOF-5. <i>Chemical Science</i> , <b>2019</b> , 10, 5906-5910   | 9.4  | 11 |
| 39 | Active sites in Cu-SSZ-13 deNO <sub>x</sub> catalyst under reaction conditions: a XAS/XES perspective. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012041                                 | 0.3  | 11 |
| 38 | Advanced X-ray Absorption Spectroscopy Analysis to Determine Structure-Activity Relationships for Cu-Zeolites in the Direct Conversion of Methane to Methanol. <i>ChemCatChem</i> , <b>2020</b> , 12, 2385-2405 | 5.2  | 10 |
| 37 | Comparing the Nature of Active Sites in Cu-loaded SAPO-34 and SSZ-13 for the Direct Conversion of Methane to Methanol. <i>Catalysts</i> , <b>2020</b> , 10, 191   | 4    | 9  |
| 36 | Pd hydride and carbide studied by means of Pd K-edge X-ray absorption near-edge structure analysis. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , <b>2015</b> , 79, 1180-1185                   | 0.4  | 9  |

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|----|---|-----|---|
| 35 | Time-dependent carbide phase formation in palladium nanoparticles. <i>Radiation Physics and Chemistry</i> , <b>2020</b> , 175, 108079   | 2.5 | 9 |
| 34 | CO <sub>2</sub> hydrogenation to methanol and hydrocarbons over bifunctional Zn-doped ZrO <sub>2</sub> /zeolite catalysts. <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 1249-1268  | 5.5 | 8 |
| 33 | Bimetallic hexanuclear clusters in Ce/Zr-UiO-66 MOFs: in situ FTIR spectroscopy and modelling insights. <i>Dalton Transactions</i> , <b>2020</b> , 49, 5794-5797  | 4.3 | 7 |
| 32 | Cerium(III) Nitrate Derived CeO <sub>2</sub> Support Stabilising PtOx Active Species for Room Temperature CO Oxidation. <i>ChemCatChem</i> , <b>2020</b> , 12, 1413-1428  | 5.2 | 7 |
| 31 | Atomic and electronic structure of free niobium nanoclusters: Simulation of the M <sub>4,5</sub> -XANES spectrum of Nb <sup>13+</sup> . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , <b>2014</b> , 195, 189-194                            | 1.7 | 6 |
| 30 | A XAFS study of the local environment and reactivity of Pt- sites in functionalized UiO-67 MOFs. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012125   | 0.3 | 6 |
| 29 | Experimental and theoretical study of hydrogen desorption process from Mn(BH <sub>4</sub> ) <sub>2</sub> . <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 735, 277-284  | 5.7 | 6 |
| 28 | Cu-Exchanged Ferrierite Zeolite for the Direct CH <sub>4</sub> to CH <sub>3</sub> OH Conversion: Insights on Cu Speciation from X-Ray Absorption Spectroscopy. <i>Topics in Catalysis</i> , <b>2019</b> , 62, 712-723   | 2.3 | 5 |
| 27 | X-ray absorption spectroscopy determination of the products of manganese borohydride decomposition upon heating. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , <b>2015</b> , 79, 139-143  | 0.4 | 5 |
| 26 | Local structure of Cu(I) ions in the MOR zeolite: A DFT-assisted XAS study. <i>Radiation Physics and Chemistry</i> , <b>2020</b> , 175, 108111  | 2.5 | 5 |
| 25 | Wavelet analysis of a Cu-oxo zeolite EXAFS simulated spectrum. <i>Radiation Physics and Chemistry</i> , <b>2020</b> , 175, 108333   | 2.5 | 5 |
| 24 | Hydrogenation of ethylene over palladium: evolution of the catalyst structure by operando synchrotron-based techniques. <i>Faraday Discussions</i> , <b>2021</b> , 229, 197-207   | 3.6 | 5 |
| 23 | Probing Structure and Reactivity of Metal Centers in Metal-Organic Frameworks by XAS Techniques <b>2017</b> , 397-430   |     | 4 |
| 22 | Doped CdTe-based quantum dots. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , <b>2015</b> , 79, 1413-1416  |     | 4 |
| 21 | Cu- and Fe-speciation in a composite zeolite catalyst for selective catalytic reduction of NO <sub>x</sub> : insights from operando XAS. <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 846-860  | 5.5 | 4 |
| 20 | Investigation of the nanoscale two-component ZnS-ZnO heterostructures by means of HR-TEM and X-ray based analysis. <i>Journal of Solid State Chemistry</i> , <b>2018</b> , 262, 264-272   | 3.3 | 3 |
| 19 | X-ray absorption spectroscopy data during formation of active Pt- and Pd-sites in functionalized UiO-67 metal-organic frameworks. <i>Data in Brief</i> , <b>2019</b> , 25, 104280   | 1.2 | 3 |
| 18 | Influence of Cu-speciation in mordenite on direct methane to methanol conversion: Multi-Technique characterization and comparison with NH <sub>3</sub> selective catalytic reduction of NO <sub>x</sub> . <i>Catalysis Today</i> , <b>2021</b> , 369, 105-111 | 5.3 | 3 |

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|----|--|-----|---|
| 17 | Hampered PdO Redox Dynamics by Water Suppresses Lean Methane Oxidation over Realistic Palladium Catalysts. <i>ChemCatChem</i> , <b>2021</b> , 13, 3765-3771  | 5.2 | 3 |
| 16 | Investigating the role of Cu-oxo species in Cu-nitrate formation over Cu-CHA catalysts. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 18322-18337   | 3.6 | 3 |
| 15 | In situ X-ray absorption study of Cu species in Cu-CHA catalysts for NH <sub>3</sub> -SCR during temperature-programmed reduction in NO/NH <sub>3</sub> . <i>Research on Chemical Intermediates</i> , <b>2021</b> , 47, 357-375    | 2.8 | 3 |
| 14 | Speciation of Ru Molecular Complexes in a Homogeneous Catalytic System: Fingerprint XANES Analysis Guided by Machine Learning. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 27844-27852                             | 3.8 | 3 |
| 13 | Spectroscopic Methods in Catalysis and Their Application in Well-Defined Nanocatalysts. <i>Studies in Surface Science and Catalysis</i> , <b>2017</b> , 221-284  | 1.8 | 2 |
| 12 | Nanotribology of copper clusters. <i>Nanotechnologies in Russia</i> , <b>2016</b> , 11, 593-602  | 0.6 | 2 |
| 11 | Spin-State Transition, Magnetism and Local Crystal Structure in Eu <sub>1-x</sub> Ca <sub>x</sub> CoO <sub>3</sub> . <i>Journal of the Physical Society of Japan</i> , <b>2013</b> , 82, 044714                                    | 1.5 | 2 |
| 10 | XAS on Rh and Ir metal sites in post synthetically functionalized UiO-67 Zirconium MOFs. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012053  | 0.3 | 2 |
| 9  | Versatile and high temperature spectroscopic cell for operando fluorescence and transmission x-ray absorption spectroscopic studies of heterogeneous catalysts. <i>Review of Scientific Instruments</i> , <b>2021</b> , 92, 023106 | 1.7 | 2 |
| 8  | Quantification of Adsorbates by X-ray Absorption Spectroscopy: Getting TGA-like Information for Free. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 5175-5179  | 3.8 | 2 |
| 7  | Investigation of oxygen vacancies in CeO <sub>2</sub> /Pt system with synchrotron light techniques. <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 712, 012064   | 0.3 | 1 |
| 6  | Kinetics of the Atomic Structure of Palladium Nanoparticles during the Desorption of Hydrogen According to X-Ray Diffraction. <i>JETP Letters</i> , <b>2019</b> , 109, 594-599   | 1.2 | 1 |
| 5  | Energy and Environmental Science at ESRF. <i>Synchrotron Radiation News</i> , <b>2020</b> , 33, 40-51  | 0.6 | 1 |
| 4  | Nanostructured Materials <b>2016</b> , 809-827   |     | 1 |
| 3  | DFT-assisted XANES simulations to discriminate different monomeric CuII species in CHA catalysts. <i>Radiation Physics and Chemistry</i> , <b>2020</b> , 175, 108510   | 2.5 | 1 |
| 2  | Photoactivated Osmium Arene Anticancer Complexes. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 17450-17461   | 5.1 | 1 |
| 1  | SO Poisoning of Cu-CHA deNO Catalyst: The Most Vulnerable Cu Species Identified by X-ray Absorption Spectroscopy.. <i>Jacs Au</i> , <b>2022</b> , 2, 787-792   |     | 0 |