# Andrey G Lyalin

List of Publications by Year
in descending order

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| 78 | 2,346 | 230014 | 252626 |
|---|---|---|---|
| papers | citations | 27 h-index | 46 g-index |

| 79 | 79 | 79 | 3004 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Catalytic Oxidative Dehydrogenation of Light Alkanes over Oxygen Functionalized Hexagonal Boron Nitride. ChemistrySelect, 2022, 7, . | 0.7 | 1 |
| 2 | Boron nitride for enhanced oxidative dehydrogenation of ethylbenzene. Journal of Energy Chemistry, 2021, 57, 477-484. | 7.1 | 23 |
| 3 | Electronic structure of the [Ni(Salen)] complex studied by core-level spectroscopies. Physical Chemistry Chemical Physics, 2021, 23, 11015-11027. | 1.3 | 7 |
| 4 | Heterocyclic Ringâ€Opening of Nanographene on Au(111). Angewandte Chemie, 2021, 133, 9513-9518. | 1.6 | 2 |
| 5 | Heterocyclic Ringâ€Opening of Nanographene on Au(111). Angewandte Chemie - International Edition, 2021, 60, 9427-9432. | 7.2 | 15 |
| 6 | Honeycomb Boron on Al(111): From the Concept of Borophene to the Two-Dimensional Boride. ACS Nano, 2021, 15, 15153-15165. | 7.3 | 20 |
| 7 | Catalytic Functionalization of Hexagonal Boron Nitride for Oxidation and Epoxidation Reactions by Molecular Oxygen. Journal of Physical Chemistry C, 2021, 125, 19219-19228. | 1.5 | 2 |
| 8 | Catalytic Activity of Gold Clusters Supported on the h-BN/Au(111) Surface for the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2021, 125, 1334-1344. | 1.5 | 17 |
| 9 | Structural Characterization of Nickel-Doped Aluminum Oxide Cations by Cryogenic Ion Trap Vibrational Spectroscopy. Journal of Physical Chemistry A, 2021, 125, 9527-9535. | 1.1 | 4 |
| 10 | Observations and theories of quantum effects in proton transfer electrode processes. Current Opinion in Electrochemistry, 2020, 19, 96-105. | 2.5 | 16 |
| 11 | Soft X-ray Li-K and Si-L2, 3 Emission from Crystalline and Amorphous Lithium Silicides in Lithium-Ion Batteries Anode. Journal of the Electrochemical Society, 2019, 166, A5362-A5368. | 1.3 | 3 |
| 12 | Single-Phase Borophene on Ir(111): Formation, Structure, and Decoupling from the Support. ACS Nano, 2019, 13, 14511-14518. | 7.3 | 99 |
| 13 | Combined Automated Reaction Pathway Searches and Sparse Modeling Analysis for Catalytic Properties of Lowest Energy Twins of Cu<sub>13</sub>. Journal of Physical Chemistry A, 2019, 123, 210-217. | 1.1 | 18 |
| 14 | CO<sub>2</sub> Adsorption on Ti<sub>3</sub>O<sub>6</sub><sup>â€“</sup>: A Novel Carbonate Binding Motif. Journal of Physical Chemistry C, 2019, 123, 8439-8446. | 1.5 | 19 |
| 15 | Lithiation Products of a Silicon Anode Based on Soft X-ray Emission Spectroscopy: A Theoretical Study. Journal of Physical Chemistry C, 2018, 122, 11096-11108. | 1.5 | 8 |
| 16 | Oxygen Reduction Reaction Catalyzed by Small Gold Cluster on h-BN/Au(111) Support. Electrocatalysis, 2018, 9, 182-188. | 1.5 | 14 |
| 17 | Quantum-to-Classical Transition of Proton Transfer in Potential-Induced Dioxygen Reduction. Physical Review Letters, 2018, 121, 236001. | 2.9 | 38 |
| 18 | Microscopic Electrode Processes in the Four-Electron Oxygen Reduction on Highly Active Carbon-Based Electrocatalysts. ACS Catalysis, 2018, 8, 8162-8176. | 5.5 | 54 |

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|---|---|---|---|
| 19 | Isomerization in Gold Clusters upon O<sub>2</sub> Adsorption. Journal of Physical Chemistry C, 2017, 121, 2661-2668. | 1.5 | 27 |
| 20 | Interface Effects in Hydrogen Elimination Reaction from Isopropanol by Ni<sub>13</sub> Cluster on Î³-Al<sub>2</sub>O<sub>3</sub>(010) Surface. Journal of Physical Chemistry C, 2017, 121, 3488-3495. | 1.5 | 13 |
| 21 | Two-Dimensional Corrugated Porous Carbon-, Nitrogen-Framework/Metal Heterojunction for Efficient Multielectron Transfer Processes with Controlled Kinetics. ACS Nano, 2017, 11, 1770-1779. | 7.3 | 50 |
| 22 | Excess charge driven dissociative hydrogen adsorption on Ti<sub>2</sub>O<sub>4</sub><sup>â”</sup>. Physical Chemistry Chemical Physics, 2017, 19, 23154-23161. | 1.3 | 16 |
| 23 | Atomically Thin Hexagonal Boron Nitride Nanofilm for Cu Protection: The Importance of Film Perfection. Advanced Materials, 2017, 29, 1603937. | 11.1 | 63 |
| 24 | When Inert Becomes Active: A Fascinating Route for Catalyst Design. Chemical Record, 2016, 16, 2324-2337. | 2.9 | 22 |
| 25 | Highly Efficient Electrochemical Hydrogen Evolution Reaction at Insulating Boron Nitride Nanosheet on Inert Gold Substrate. Scientific Reports, 2016, 6, 32217. | 1.6 | 72 |
| 26 | Gold nanoparticle decoration of insulating boron nitride nanosheet on inert gold electrode toward an efficient electrocatalyst for the reduction of oxygen to water. Electrochemistry Communications, 2016, 66, 53-57. | 2.3 | 35 |
| 27 | Long Range Functionalization of h-BN Monolayer by Carbon Doping. Journal of Physical Chemistry C, 2016, 120, 15993-16001. | 1.5 | 42 |
| 28 | Reactivity of Gold Clusters in the Regime of Structural Fluxionality. Journal of Physical Chemistry C, 2015, 119, 11120-11130. | 1.5 | 40 |
| 29 | From Graphene Nanoribbons on Cu(111) to Nanographene on Cu(110): Critical Role of Substrate Structure in the Bottom-Up Fabrication Strategy. ACS Nano, 2015, 9, 8997-9011. | 7.3 | 127 |
| 30 | Adsorption and Catalytic Activation of the Molecular Oxygen on the Metal Supported h-BN. Topics in Catalysis, 2014, 57, 1032-1041. | 1.3 | 34 |
| 31 | Application of Automated Reaction Path Search Methods to a Systematic Search of Single-Bond Activation Pathways Catalyzed by Small Metal Clusters: A Case Study on Hâ€“H Activation by Gold. Journal of Chemical Theory and Computation, 2014, 10, 1623-1630. | 2.3 | 28 |
| 32 | Boron Nitride Nanosheet on Gold as an Electrocatalyst for Oxygen Reduction Reaction: Theoretical Suggestion and Experimental Proof. Journal of the American Chemical Society, 2014, 136, 6542-6545. | 6.6 | 231 |
| 33 | Oxygen activation and dissociation on hâ€BN supported Au atoms. International Journal of Quantum Chemistry, 2013, 113, 443-452. | 1.0 | 39 |
| 34 | Functionalization of Monolayer h-BN by a Metal Support for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2013, 117, 21359-21370. | 1.5 | 109 |
| 35 | Theoretical predictions for hexagonal BN based nanomaterials as electrocatalysts for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2013, 15, 2809. | 1.3 | 95 |
| 36 | CO oxidation on h-BN supported Au atom. Journal of Chemical Physics, 2013, 138, 034701. | 1.2 | 71 |

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| 37 | The h-BN surface effect on CO oxidation reaction catalyzed by supported gold atom. Journal of Physics: Conference Series, 2013, 438, 012003. | 0.3 | 4 |
| 38 | Catalytic Activity of Au and Au<sub>2</sub> on the h-BN Surface: Adsorption and Activation of O<sub>2</sub>. Journal of Physical Chemistry C, 2012, 116, 9054-9062. | 1.5 | 84 |
| 39 | A computational investigation of H2 adsorption and dissociation on Au nanoparticles supported on TiO2 surface. Faraday Discussions, 2011, 152, 185. | 1.6 | 54 |
| 40 | Role of the Support Effects on the Catalytic Activity of Gold Clusters: A Density Functional Theory Study. Catalysts, 2011, 1, 18-39. | 1.6 | 38 |
| 41 | Adsorption of Ethylene on Neutral, Anionic, and Cationic Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 2484-2493. | 1.5 | 61 |
| 42 | Reactant-Promoted Oxygen Dissociation on Gold Clusters. Journal of Physical Chemistry Letters, 2010, 1, 1752-1757. | 2.1 | 75 |
| 43 | Impurity effect on the melting of nickel clusters as seen via molecular dynamics simulations. Physical Review B, 2009, 79, . | 1.1 | 34 |
| 44 | Cooperative Adsorption of O<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> on Small Gold Clusters. Journal of Physical Chemistry C, 2009, 113, 12930-12934. | 1.5 | 53 |
| 45 | Catalitic Activity of Gold Clusters. AIP Conference Proceedings, 2009, , . | 0.3 | 5 |
| 46 | Droplet model of an atomic cluster at a solid surface. Journal of Experimental and Theoretical Physics, 2008, 106, 678-689. | 0.2 | 14 |
| 47 | SIMULATION OF THE NANOINDENTATION PROCEDURE ON PURE NICKEL ON THE SMALLEST LENGTH SCALE: A SIMPLE ATOMISTIC LEVEL MODEL. , 2008, , 205-224. | | 0 |
| 48 | Interplay of electronic and geometry shell effects in properties of neutral and charged Sr clusters. Physical Review A, 2007, 75, . | 1.0 | 19 |
| 49 | Structure and magnetism of lanthanum clusters. Physical Review A, 2006, 74, . | 1.0 | 43 |
| 50 | Polarizational bremsstrahlung from atomic clusters. Radiation Physics and Chemistry, 2006, 75, 1358-1379. | 1.4 | 8 |
| 51 | FISSION OF METAL CLUSTERS. International Journal of Modern Physics E, 2006, 15, 153-195. | 0.4 | 12 |
| 52 | Dissociation and fission of small sodium and strontium clusters. European Physical Journal D, 2005, 34, 93-96. | 0.6 | 6 |
| 53 | Geometrical and statistical factors in fission of small metal clusters. Physical Review B, 2005, 72, . | 1.1 | 8 |
| 54 | Stability of small neutral and charged strontium clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, L129-L135. | 0.6 | 9 |

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| 55 | Rearrangement of cluster structure during fission processes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, L7-L13. | 0.6 | 6 |
| 56 | Molecular Dynamics Simulations of Cluster Fission and Fusion Processes. Physica Scripta, 2004, 110, 319. | 1.2 | 5 |
| 57 | METAL CLUSTER FISSION: JELLIUM MODEL AND MOLECULAR DYNAMICS SIMULATIONS. , 2004, , 157-168. | | 2 |
| 58 | AB INITIO CALCULATIONS AND MODELLING OF ATOMIC CLUSTER STRUCTURE. , 2004, , 51-65. | | 0 |
| 59 | On the applicability of deformed jellium model to the description of metal clusters. European Physical Journal D, 2003, 24, 15-18. | 0.6 | 7 |
| 60 | Evolution of the electronic and ionic structure of Mg clusters with increase in cluster size. Physical Review A, 2003, 67, . | 1.0 | 112 |
| 61 | ON THE APPLICABILITY OF THE JELLIUM MODEL TO THE DESCRIPTION OF ALKALI CLUSTERS. International Journal of Modern Physics E, 2003, 12, 81-107. | 0.4 | 21 |
| 62 | METAL CLUSTER FISSION. , 2003, , . | | 0 |
| 63 | Hartree-Fock approach for metal-cluster fission. Physical Review A, 2002, 65, . | 1.0 | 9 |
| 64 | Comparative study of metal-cluster fission in Hartree-Fock and local-density approximations. Physical Review A, 2002, 65, . | 1.0 | 20 |
| 65 | A relativistic description of the polarization mechanism of elastic bremsstrahlung. Journal of Experimental and Theoretical Physics, 2002, 94, 704-719. | 0.2 | 12 |
| 66 | Hartreeâ€Fock Deformed Jellium Calculations for Metallic Clusters. Journal of the Chinese Chemical Society, 2001, 48, 419-426. | 0.8 | 8 |
| 67 | A simple atomic model for hydrogen confined inside a prolate-shaped C60fullerene cage. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2505-2511. | 0.6 | 25 |
| 68 | Hartree-Fock deformed jellium model for metallic clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 3653-3664. | 0.6 | 24 |
| 69 | Manifestation of the Bethe ridge in the polarizational bremsstrahlung process. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, L179-L186. | 0.6 | 2 |
| 70 | The role of the polarization mechanism for emission of radiation by atoms over a broad photon frequency range. Journal of Experimental and Theoretical Physics, 1998, 87, 251-259. | 0.2 | 15 |
| 71 | Total bremsstrahlung spectra of 1 - 25 keV electrons on Ne and Ar. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, L115-L121. | 0.6 | 20 |
| 72 | Theoretical treatment of the bremsstrahlung process in the vicinity of giant atomic resonances. Physical Review A, 1996, 53, 2230-2238. | 1.0 | 8 |

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| 73 | Semi-empirical method for polarizational bremsstrahlung calculation. Journal of Electron Spectroscopy and Related Phenomena, 1996, 79, 323-326. | 0.8 | 5 |
| 74 | Electron bremsstrahlung spectra on La near the 4d threshold. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, L611-L617. | 0.6 | 6 |
| 75 | Bremsstrahlung Emission in Collisions of Electrons with Atoms and Clusters. , 1996, , 263-278. | | 1 |
| 76 | New method for the polarizational bremsstrahlung calculation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 4947-4962. | 0.6 | 19 |
| 77 | Theoretical treatment of bremsstrahlung spectra in the vicinity of giant atomic resonances: application to Ba. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, L155-L160. | 0.6 | 17 |
| 78 | Superior Multielectronâ€Transferring Energy Storage by Ï€â€d Conjugated Frameworks. Small, 0, , 2202861. | 5.2 | 1 |