Ilia V. Chepkasov

Curriculum Vitae

PERSONAL DATA

Affiliation Research Scientist, Skolkovo Institute of Science and Technology, Moscow, Russia
Date of birth October 5, 1988
E-mail I.Chepkasov@skoltech.ru
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URL https://scholar.google.ru/citations?user=uld736gAAAAJ&hl=ru
https://www.researchgate.net/profile/Ilya_Chepkasov2

RESEARCH INTERESTS

nanoparticles, gas-phase condensation, thermodynamic properties of nanoalloy, electron properties of nanoalloy, catalytic properties of nanoalloy, 2D material, DFT, MD, machine learning interatomic potentials, global optimization.

OTHER SKILLS

Scientific programs: VMD, Ovito, Origin, VESTA, Python, LAMMPS, DL_POLY, OpenMX, VASP, QuantumATK, USPEX, Phonopy, Lobster, MLIP.

EMPLOYMENT and POSITIONS

08/2020 -present Skolkovo Institute of Science and Technology, Moscow, Russia
research scientist, Center for Energy Science and Technology
03/2021 --09/2021 Helmholtz-Zentrum Dresden-Rossendorf Dresden, Germany
visiting researcher at the Atomistic simulations of irradiation-induced phenomena
06/2019 -08/2020 National University of Science and Technology "MISIS", Moscow, Russia
visiting researcher at the Inorganic Nanomaterial Laboratory
10/2018 -03/2019 Helmholtz-Zentrum Dresden-Rossendorf Dresden, Germany
visiting researcher at the Atomistic simulations of irradiation-induced phenomena
1/2014 – 10/2018 Katanov Khakas State University Abakan, Russia
researcher at the Nanophysics Laboratory
6/2014 – 08/2020 Katanov Khakas State University Abakan, Russia
assistant professor at the Department of Physics
9/2012 – 12/2012 Institute of Metallurgy of the Ural Branch of the RAS Ekaterinburg, Russia
junior researcher at the Group of RAS Advisor (Internship)

EDUCATION and DEGREES

10/2010-11/2013 Katanov Khakas State University Abakan, Russia
PhD student, 20.11.2013 - Candidate of Physico-Mathematical Sciences (Equivalent to Ph.D., Condensed Matter Physics). Thesis: Molecular dynamics simulations synthesis of Cu nanoparticles from the gas phase
(Supervisor: Yuri Ya. Gafner, yurigafner@gmail.com)
9/2005 – 8/2010 Katanov Khakas State University Abakan, Russia
Basic classical education, Physics

ADVANCED SCHOOLS

2/2014-3/2014 Forschungszentrum Jülich, Peter Grünberg Institute Jülich, Germany
45th IFF Spring School "Computing Solids: Models, Ab-initio Methods and Supercomputing"
3/2015 Forschungszentrum Jülich, Peter Grünberg Institute Jülich, Germany
46th IFF Spring School "Functional Soft Matter"
3/2019 Forschungszentrum Jülich, Peter Grünberg Institute Jülich, Germany
46th IFF Spring School "Scattering! Soft, Functional and Quantum Materials"

AWARDS and PRIZES

2016 The third place for the report at the XIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia

2012-2013	Special state scholarship of Russian Federation Government 2012/13. The Order of Ministry of Education and Science of the Russian Federation №935 from 19.11.2012
2012	Certificate for the best report at the XVIII Russian conference of students and young scientists physicists (VNKSF-18), Siberian Federal University, Krasnoyarsk, Russia
2012	Award of the Government of the Republic of Khakassia in the category "Young researcher"
2011	The first place for the report at the VIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia
2010	The first place in the Republican competition of scientific – research works of students of higher educational institutions, Abakan, Russia
2010	Russian President Student Award for supporting talented young students.
2010	Award of the Government of the Republic of Khakassia in the category "Young researcher", Abakan, Russia
2009	The first place in the Republican competition of scientific – research works of students of higher educational institutions, Abakan, Russia

GRANT HELD

1. Russian Science Foundation (Project 22-73-00219) [2022-2024]: «Computer design of new electrolytes for solid-state batteries», **Principal Investigator.** (Russia)
2. German Academic Exchange Service- DAAD program "Mikhail Lomonosov" [2020-2021]: «*Prospective materials for the anodes of high-capacity metal-ion batteries from first-principles computer simulations* », **Principal Investigator**. (Germany)
3. German Academic Exchange Service- DAAD program "Mikhail Lomonosov" [2018-2019]: «*Atomistic simulations of impacts of high-energy ions on two-dimensional transition metal dichalcogenides within the framework of a two-temperature model*», **Principal Investigator**. (Germany)
4. Program of Foundation for promoting the development of small enterprises in scientific and technical sphere, *UMNIK* program [2017-2018]: «*Development of a software package for optimization of synthesis parameters for nanopowders of metals and alloys*», **Principal Investigator**. (Russia)
5. Prokhorov Foundation grant, «*Academic Mobility*» program [2017], **Principal Investigator**. (Russia)
6. Grant of Russian Foundation for Basic Research (Russia)
   a. [2017-2018], #17-42-190308_r: «*Complex experimental and theoretical investigation of iron and manganesesilicides epitaxial thin films* », **Principal Investigator**;
   b. [2016-2017], #16-48-190182_r:«*Development of some technological aspects for creation stable metal nanoobjects and some technical devices on their basis*»**,** co-P.I.;
   c. [2016-2017], #16-32-000125-mol_a: «*Investigation of synthesis mechanisms and thermal properties of homogeneous and heterogenous bicomponent nanoparticles*», **Principal Investigator**;
   d. [2015-2016], #15-42-04164_r_sibir'_a: «*Creation of the ordered structures from nanodispersed particles condensed from a gas phase*», co-P.I.;
   e. [2013-2014], #13-02-98000_r_sibir'_a: «*Creation of experimental-theoretical bases for synthesis of nanopowders of metals, oxides, nitrides synthesized after condensation of high temperature vapor*», co-P.I.;
   f. [2012-2013], #12-02-98000_r_sibir'_a: «*Development of the theory for creation stable nanostructures on the basis of metal clusters under condition of external influence various nature*», co-P.I.;
   g. [2012], #12-02-90804-mol_rf_nr: «*The thermal stability of ensembles of nanoclusters Ir and RuonSiO2 substrate and grapheme*», **Principal Investigator**;
   h. [2011-2012], #11-02-98006_r_sibir'_a: «*Creation of theoretical bases for synthesis of metal nanoparticles from the gas environment*», co-P.I.;
   i. [2009-2010], #09-02-98000_r_sibir'_a: «*Development of the theory of metal nanoparticles synthesis from a high-temperature gas phase*», co-P.I.;
7. Grants of the President of Russian Federation [2009-2010], # MK_2207.2009.2: «*The development of physical and technological principles of formation of nanostructures of certain fcc metals for the catalysis and functional electronics*», co-P.I.; (Russia)
8. State Task of the Ministry of Education and Science of the Russian Federation [2014-2016]: «*Computer modeling of the theoretical foundations of the production of nanostructures of fcc metals, stable, subject to various external influences*» co-P.I.; (Russia)

WORKSHOPS and CONFERENCES (PROFESSIONAL and SCIENTIFIC MEETING)

9/2019 Inaugural Symposium for Computational Materials Program of Excellence (CMP Symposium), Skoltech, Moscow, Russia

6/2019 Workshop «Application of Machine-Learning Interatomic Potentials in Materials Design», Moscow, Russia

5/2019 Physics Boat Workshops (PBW - 2019), poster session «Atomic structure and electronic properties of few-atom alkali metal between two graphene and MoS_2 sheets», Helsinki, Finland - Stockholm, Sweden

3/2019 50th IFF Spring School Scattering! Soft, Functional and Quantum Materials, poster session, «Atomic structure and electronic properties of few-atom Li, Na, K layers between two graphene and MoS_2 sheets», Jülich, Germany

2/2019 Towards Reality in Nanoscale Materials X, poster session, «Atomic structure and electronic properties of few-atom sodium and potassium layers between two graphene sheets», Levi, Finland.

8/2018 XXVII International Materials Research Congress, «Computer investigation of synthesis, structural and electronic properties of bimetallic nanoparticles» **Invited Speaker**, Cancun, Mexico.

3/2017 Seminar «Computer simulation of nanoparticles», Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russia

4/2016 XIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia

6/2016 International Scientific and Technical Conference Nanotechnologies of Functional Materials (NFM'16), Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia

2/2015 Seminar Laboratory of Physics of the magnetic phenomena «Theoretical modeling of thermal effects on the copper nanoparticles», L.V. Kirensky Institute of Physics, Krasnoyarsk, Russia

9/2014 IV Interdisciplinary International Symposium «The physics of surface phenomena, phase boundaries and phase transitions» (PSP&PT), Tuapse, Russia

11/2012 All-Russian Youth Conference «Physics and chemistry of nanoscale systems», Ural Federal University, Ekaterinburg, Russia

3/2012 XVIII Russian conference of students and young scientists physicists (VNKSF-18), Siberian Federal University, Krasnoyarsk, Russia

9/2011 XIII International Conference «Opto, nanoelectronics, nanotechnologies and microsystems», Ulyanovsk State University, Abrau-Durso, Russia

6/2011 9th International Scientific Conference «Advanced metal materials and technologies» (AMMT'2011), Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia

4/2011 VIII International Conference of Students and Young Scientists «Prospects of Fundamental Sciences Development», National Research Tomsk Polytechnic University, Tomsk, Russia

11/2010 XI All-Russian School-Seminar on Physics of Condensed Matter(SPFKS-11), Institute of Metal Physics, Ekaterinburg, Russia

9/2010 XI International Workshop «Evolution of the defect structure in Condensed Matter», Altai State Technical University, Barnaul, Russia

4/2010 XLVIII International Scientific Student Conference «Student and technological progress», Novosibirsk State University, Novosibirsk, Russia

2/2010 2thAll-Russian seminar «Physics and chemistry of surfaces and nanostructures», A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS, Moscow, Russia

10/2009 X All-Russian School-Seminar on Physics of Condensed Matter(SPFKS-10), Institute of Metal Physics, Ekaterinburg, Russia

5/2009 VI International Conference of Students and Young Scientists «Prospects of Fundamental Sciences Development», National Research Tomsk Polytechnic University, Tomsk, Russia

REFEREE FOR SCIENTIFIC JOURNALS

Journal of Alloys and Compounds, Industrial & Engineering Chemistry Research, Journal of Molecular Liquids, Computational Materials Science

PUBLICATIONS

1. Leybo D, Firestein K.L., Evdokimenko N.D., Ryzhova A.A., Baidyshev V.S., **Chepkasov I.V.**, Popov Z.I., Kustov A.L., Konopatsky A.S., Golberg D.V., Shtansky D. V. Effect of ball-mill processing on catalytic activity and selectivity of Fe/h-BN catalysts for CO_2 hydrogenation // ACS Applied Nano Materials 2022 (in the press)
2. **Chepkasov I. V.**, Baidyshev V. S., Golubnichiy A. A., Zamulin I. S., Kvashnin A. G., Kozlov S. M. Cu–Au nanoparticles produced by the aggregation of gas-phase metal atoms for CO oxidation // Aggregate 2022, e273. https://doi.org/10.1002/agt2.273

3. **Chepkasov I. V.**, Smet J. H., Krasheninnikov A. V. Single-and Multilayers of Alkali Metal Atoms inside Graphene/MoS_2 Heterostructures: A Systematic First-Principles Study //The Journal of Physical Chemistry C. 2022, 126, 37, 15558–15564
4. Rybin N., **Chepkasov I.V.**, Novoselov D. Y., Anisimov V. I., Oganov A. R Prediction of Stable Silver Fluorides //The Journal of Physical Chemistry C. 2022, 126, 35, 15057–15063.
5. Kvashnin A. G., Nikitin D. S., Shanenkov I. I., **Chepkasov I. V.**, Kvashnina Y. A., Nassyrbayev, A., Sivkov A. A., Bolatova Z., Pak A. Ya. Large-Scale Synthesis and Applications of Hafnium–Tantalum Carbides // Advanced Functional Materials. 2022. 2206289. (Q1)
6. Wang, Y., Bykov, M., **Chepkasov, I.V.**, Samtsevich, A., Bykova, E., Zhang, X., Jiang S., Greenberg E., Chariton S., Prakapenka V. B. , OganovA. R., Goncharov, A. F. Stabilization of hexazine rings in potassium polynitride at high pressure //Nature Chemistry. 2022. 14. 794–800 (Q1)
7. Kovalskii A. M., Volkov I. N., Evdokimenko N. D., Tkachenko O. P., Leybo D. V., **Chepkasov I. V.**, Popov Z. I., Matveev A. T., Manakhov A., Permyakova E. S., Konopatsky A. S., Kustov A. L., Golberg D.V., Shtansky D. V. Hexagonal BN-and BNO-supported Au and Pt nanocatalysts in carbon monoxide oxidation and carbon dioxide hydrogenation reactions //Applied Catalysis B: Environmental. 2022. 303. 120891. (Q1)
8. **Chepkasov I. V.**, Sukhanova E. V., Kvashnin A. G., Zakaryan H. A., Aghamalyan M. A., Mamasakhlisov Y. S., Manakhov A.M., Popov Z.I., Kvashnin D. G. Computational Design of Gas Sensors Based on V_3S_4 Monolayer //Nanomaterials. 2022. 12. 5. 774. (Q1)
9. K. L. Firestein, N. D. Evdokimenko, A. L. Kustov, V. S. Baidyshev, **I. V. Chepkasov**, Z. I. Popov, A. T. Matveev, I. V. Shetinin, D. V. Leybo, I. N. Volkov, A. M. Kovalsky, D. Golberg, D. V. Shtansky Microstructure and catalytic properties of Fe3O4/BN, Fe3O4 (Pt)/BN, and FePt/BN heterogeneous nanomaterials in CO_2 hydrogenation reaction: Experimental and theoretical insights //Journal of Catalysis. 2021. 402. 130-142. (Q1)
10. **Chepkasov I. V.**, Erohin S. V., Sorokin P. B. The Features of Phase Stability of GaN and AlN Films at Nanolevel //Nanomaterials. – 2021. 11. 1. 8. (Q1)
11. **Chepkasov I. V.**, Ghorbani-Asl M., Popov Z. I., Smet J. H., Krasheninnikov A. V. Alkali metals inside bi-layer graphene and MoS_2: insights from first-principles calculations // Nano Energy. 2020. 104927. (Q1)
12. **Chepkasov I.V.**, Baidyshev V.S., Sukhanova E.V., Visotin M.A., Süle P., Popov Z.I. Iron silicides formation on Si (100) and (111) surfaces through theoretical modeling of sputtering and annealing // Applied Surface Science. 2020. 146736. (Q1)
13. Konopatsky, A.S., Leybo, D.V., Firestein, K.L., **Chepkasov, I.V.**, Popov, Z.I., Permyakova, E.S., Volkov, I.N., Kovalskii, A.M., Matveev, A.T., Shtansky, D.V., Golberg, D.V. Polyol synthesis of Ag/BN nanohybrids and their catalytic stability in CO oxidation reaction //ChemCatChem. 2020. 12. 6. 1691-1698. (Q1)
14. Ponomarev V., Sheveyko A. N., Permyakova E. S., Lee J., Voevodin A. A., Berman D, Manakhov A., Michlicek M., Slukin P., Firstova V., Ignatov S., **Chepkasov I. V.**, Popov Z. I., Shtansky D.V. TiCaPCON-Supported Pt-and Fe-based Nanoparticles and Related Antibacterial Activity // ACS Applied Materials & Interfaces 2019. 11. 32. 28699-28719(Q1)
15. **Chepkasov I. V.**, Visotin M. A., Kovaleva E. A., Manakhov A. M., Baidyshev V. S., Popov Z. I. Stability and Electronic Properties of PtPd Nanoparticles via MD and DFT Calculations //The Journal of Physical Chemistry C. 2018. 122. 31. 18070-18076.
16. Baidyshev V. S., **Chepkasov I. V.,** Artemova N. D. Study of thermal stability of disordered alloy Ag_xCu_{1-x} nanoparticles by molecular dynamic simulations //Journal of Physics: Conference Series. 2018. 1015. 3. 032021.
17. **Chepkasov I. V.**, Baidyshev V. S., Baev A. Y. Structural properties of CuAu nanoparticles with different type. Molecular dynamic simulations //Journal of Physics: Conference Series. 2018. 1015. 3. 032022.
18. **Chepkasov I. V.**, Baidyshev V. S., Tsura V. A. Molecular dynamic simulation of melting copper-silicon nanoparticles //Journal of Physics: Conference Series. 2018. 1015. 3. 032023.
19. **Chepkasov I. V.**, GafnerYu.Ya., Visotin M.A., Redel L.V. Melting of PdPt nanoparticles of different types // Physics of the Solid State. 2017. 59. 10. 2076-2081.
20. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L. Synthesis of Cu nanoparticles by condensation from the gas phase //Phase Transitions. 2017. 90. 6. 590-597.
21. Kurbanova E. D., Polukhin V. A., **Chepkasov I. V.** Thermostability of interface structure metal on graphene and silicene //Letters on materials. 2016. 6. 2. 109-112.
22. **Chepkasov I. V.,** Gafner Y. Y., Gafner S. L., Bardakhanov S. P. Condensation of Cu nanoparticles from the gas phase //The Physics of Metals and Metallography. 2016. 117. 10. 1003-1012.
23. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L. Changing of the shape and structure of Cu nanoclusters generated from a gas phase: MD simulations //Journal of Aerosol Science. 2016. 91. 33-42.
24. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L., Bardakhanov S. P. The general mechanisms of Cu cluster formation in the processes of condensation from the gas phase //Bulletin of Materials Science. 2015. 38. 3. 701-706.
25. **Chepkasov I. V.**, Popov Z. I. Analysis of thermal effects on copper nanoparticles synthesized from the gas phase //IOP Conference Series: Materials Science and Engineering. – IOP Publishing, 2015. 81. 1. 012033.

26. **Chepkasov I. V.**, Redel L. V. Calculations of the heat capacity of Cu clusters synthesized by condensation from the gas phase //IOP Conference Series: Materials Science and Engineering. – IOP Publishing. 2015. 81. 1. 012014.
27. **Chepkasov I. V.**, Gafner Yu.Ya., Gafner S.L. Role of the Clusters' Boundaries in the Calculations of the Heat Capacity of Cu Clusters Synthesized from the Gas Environment //Quantum Matter. 2014. 3. 1. 78-83.
28. **Chepkasov I. V.**, GafnerYu.Ya., Kurbanova E.D., Polukhin V.A. Study of the effect of ultrafast heating on the structure and shape of the gas phase synthesized Cu nanoparticless // Letters on materials. 2014. 4. 4. 249-252.
29. Polukhin V. A., Gafner Y. Y., **Chepkasov I. V.**, Kurbanova E. D. Comparative analysis of the thermosize effects of transition-metal clusters that are free or deposited onto graphene. Molecular dynamics simulation //Russian Metallurgy (Metally). 2014. 2014. 2. 112-125.
30. **Chepkasov I.V.**, Gafner Yu.Ya., Gafner S.L. Analysis of the impact of thermal effects on the structural evolution of nanoclusters Cu and Ni // Russian Physics Journal. 2011. 54. 1/3. 318 - 324.
31. Gafner Y. Y., Gafner S. L., **Chepkasov I. V.** The effect of thermal treatment on the organization of copper and nickel nanoclusters synthesized from the gas phase //Journal of Experimental and Theoretical Physics. 2010. 111. 4. 608-618.