 Ilia V. Chepkasov

Curriculum Vitae

**PERSONAL DATA**

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| **Affiliation** | Research Scientist, Skolkovo Institute of Science and Technology, Moscow, Russia |  |
| **Date of birth**  | October 5, 1988 |
| **E-mail****Skype** | ilya\_chepkasov@mail.ruilya\_chepkasov |
| **URL** | https://scholar.google.ru/citations?user=uld736gAAAAJ&hl=ruhttps://www.researchgate.net/profile/Ilya\_Chepkasov2 |  |

**RESEARCH INTERESTS**

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| nanoparticles, gas-phase condensation, thermodynamic properties of nanoalloy, electron properties of nanoalloy, , 2D material, DFT, MD |

**OTHER SKILLS**

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| Scientific programs: VMD, Ovito, Origin, VESTA, Python, LAMMPS, DL\_POLY, OpenMX, VASP, QuantumATK, USPEX |

**EMPLOYMENT and POSITIONS**

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| **08/2020 -present** | Skolkovo Institute of Science and Technology, | Moscow, Russia |
| research scientist, Center for Energy Science and Technology |
| **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**

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| **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 Сu nanoparticles from the gas phase(Advisor: Yuri Ya. Gafner, yurigafner@gmail.com) |
| **9/2005 – 8/2010** | Katanov Khakas State University | Abakan, Russia |
| Basic classical education, Physics |

**ADVANCED SCHOOLS**

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| **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**

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| **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](http://tpu.ru), 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](http://tpu.ru), Tomsk, Russia |
| **2010** | The first place in the Republican [competition](http://www.lingvo-online.ru/ru/Search/Translate/GlossaryItemExtraInfo?text=%d0%ba%d0%be%d0%bd%d0%ba%d1%83%d1%80%d1%81&translation=competition&srcLang=ru&destLang=en) 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](http://www.lingvo-online.ru/ru/Search/Translate/GlossaryItemExtraInfo?text=%d0%ba%d0%be%d0%bd%d0%ba%d1%83%d1%80%d1%81&translation=competition&srcLang=ru&destLang=en) of scientific – research works of students of higher educational institutions, Abakan, Russia |

**GRANT HELD**

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| 1.2. | 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)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) |
| 3.4. | 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)Prokhorov Foundation grant, «*Academic Mobility*» program [2017], **Principal Investigator**. (Russia) |
| 5. | Grant of Russian Foundation for Basic Research (Russia) |
|  | a.b. | [2017-2018], #17-42-190308\_r: «*Complex experimental and theoretical investigation of iron and manganesesilicides epitaxial thin films* », **Principal Investigator**;[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.; |
| 6. | 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 electronic*s», co-P.I.; (Russia) |
| 7. | 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)**

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| **9/2019****6/2019****5/2019****3/2019****2/2019****8/2018****3/2017****4/2016****6/2016****2/2015** | Inaugural Symposium for Computational Materials Program of Excellence (CMP Symposium), Skoltech, Moscow, RussiaWorkshop «Application of Machine-Learning Interatomic Potentials in Materials Design», Moscow, RussiaPhysics Boat Workshops (PBW - 2019), poster session «Atomic structure and electronic properties of few-atom alkali metal between two graphene and MoS2 sheets», Helsinki, Finland - Stockholm, Sweden50th 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 MoS2 sheets», Jülich, GermanyTowards 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. XXVII International Materials Research Congress, «Computer investigation of synthesis, structural and electronic properties of bimetallic nanoparticles» **Invited Speaker**, Cancun, Mexico.Seminar «Computer simulation of nanoparticles», Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russia XIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", [National Research Tomsk Polytechnic University](http://tpu.ru), Tomsk, RussiaInternational Scientific and Technical Conference Nanotechnologies of Functional Materials (NFM'16), Peter the Great St. Petersburg Polytechnic University, St. Petersburg, RussiaSeminar 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](http://tpu.ru), 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](http://tpu.ru), Tomsk, Russia |

**REFEREE FOR SCIENTIFIC JOURNALS**

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

**PUBLICATIONS**

1. **Chepkasov I. V.**, Erohin S. V., Sorokin P. B. The Features of Phase Stability of GaN and AlN Films at Nanolevel //Nanomaterials. – 2021. – Т. 11. – №. 1. – С. 8.
2. **Chepkasov I. V.**, Ghorbani-Asl M., Popov Z. I., Smet J. H., Krasheninnikov A. V. Alkali metals inside bi-layer graphene and MoS2: insights from first-principles calculations // Nano Energy. – 2020. – С. 104927.
3. **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. – С. 146736.
4. 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. – Т. 12. – №. 6. – С. 1691-1698.
5. 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. –V. 11 – № 32. – P.28699-28719
6. **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. – V. 122. – №. 31. – P. 18070-18076.
7. Baidyshev V. S., **Chepkasov I. V.,** Artemova N. D. Study of thermal stability of disordered alloy AgxCu1-x nanoparticles by molecular dynamic simulations //Journal of Physics: Conference Series. 2018. – V. 1015. – №. 3. – P. 032021.
8. **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. – V. 1015. – №. 3. – P. 032022.
9. **Chepkasov I. V.**, Baidyshev V. S., Tsura V. A. Molecular dynamic simulation of melting copper-silicon nanoparticles //Journal of Physics: Conference Series. 2018. – V. 1015. – №. 3. – P. 032023.
10. **Chepkasov I. V.**, GafnerYu.Ya., Visotin M.A., Redel L.V. Melting of PdPt nanoparticles of different types // Physics of the Solid State. – 2017. – V.59. - № 10 – P. 2076-2081.
11. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L. Synthesis of Cu nanoparticles by condensation from the gas phase //Phase Transitions. – 2017. – V. 90. – №. 6. – P. 590-597.
12. Kurbanova E. D., Polukhin V. A., **Chepkasov I. V.** Thermostability of interface structure metal on graphene and silicene //Letters on materials. – 2016. – V. 6. – №. 2. – P. 109-112.
13. **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. – V. 117. – №. 10. – P. 1003-1012.
14. **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. – V. 91. – P. 33-42.
15. **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. – V. 38. – №. 3. – P. 701-706.
16. **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. – V. 81. – №. 1. – P. 012033.
17. **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. – V. 81. – №. 1. – P. 012014.
18. **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. – V. 3. – №. 1. – P. 78-83.
19. **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. – V. 4. – №. 4. – P. 249-252.
20. 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. – V. 2014. – №. 2. – P. 112-125.
21. **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. – V. 54. - № 1/3. – P. 318 - 324.
22. 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. – V. 111. – №. 4. – P. 608-618.