Alexey Kartsev

Curriculum Vitae

Romana Bryanskogo 5/1
24103 Bryansk, Russia
+7 (909) 915-04-70
kartsev.alexey@aol.com

Info

Born	October, 20 1985; Bryansk, Russia	Citizenship	Russian
Add. e-mail	alexey@teorfys.lu.se	Skype	karec1
Web page	http://matfys.lth.se/staff/Alexey.Kartsev	LinkedIn	LinkedIn profile
ResearchGate	ResearchGate	GoogleScholar	Google scholar

Education and Experience

2002-2008 **Master Degree in Condensed Matter Physics**, *National University of Science and Technology "MISIS"*, Moscow, Russia.
I have completed the 6 year program at the Theoretical Physics department at National University of Science and Technology. During last four years I had been focusing more on specialized areas. I received unique knowledge about real materials and physicochemical properties thereof. Supervisor Prof. Vekilov Yu. Kh. Co-supervisor Prof. E.I. Isaev.

2008 **Department Assistant**, *National University of Science and Technology "MISIS"*, Moscow, Russia.
Teaching and field trip escorting of students. Research activity.

2008-2013 **PhD in Theoretical Physics**, *Lund University*, Lund, Sweden.
I have earned a PhD degree in physics at the Mathematical Physics Department of Lund University. My studies were focused on numerical methods and condensed matter simulations using Time Dependent Density Functional Theory calculations on a supercomputer clusters. The research was carried out in collaboration with U.S. air force base Kirtland and Sandia National Laboratory `http://www.dtic.mil/cgi-bin/GetTRDoc?AD=ADA566596`
Supervisor Prof. Claudio Verdozzi. Co-supervisor Prof. Carl-Olof Almbladh
Thesis opponent: Prof. Irene D'Amico.

2013-2014 **Researcher**, *Uppsala University*, Uppsala, Sweden.
TDDFT project activity in the Division of Materials Theory supervised by Olle Eriksson.

2015-2016 **Postdoc**, *CEA DSM/IRAMIS/SPEC*, Saclay-Paris, France.
Electronic transport in magnetic nanostructures and molecular spintronics. Work was done in close collaboration with senior group members: Alexander Smogunov and Cyrille Barreteau.

2014-present **Researcher**, *Interdisciplinary Laboratory of Computer Modeling and Condensed Matter Analysis, Tomsk State University*, Tomsk, Russia.
Electronic structure problems for condensed crystalline systems. Igor Abrikosov group.

Specialization and current research interests

Solid State Physics | Electronic Theory of Solids | Scientific Programming

Lattice Dynamic | Density Functional Theory

Strongly Correlated Systems | Hubbard Model | UltraCold Atoms

Exact static and time-dependent methods | Numerical solution of model Hamiltonians

Research Projects

2007-2008 *Ab initio* simulation of electronic, structural properties and lattice dynamics of magnetic metal mononitrides

2008-2009 Numerical solution of 1D Bethe-Ansatz equation for the new DFT *xc* potential in the Hubbard cluster

2009-2011 Numerical study of magnetic 1D Fermi gas in the optical lattice using TDDFT

2011 Transport through a single level quantum dot connected to semi-infinite leads

2010-2013 Expansion and collision of trapped fermionic clouds in 3D optical lattice

2013-2014 Cr-base high temperature alloys

2015 Molecules on the metal substrates in the presence of electron-vibron coupling and molecules with controlled magnetic states

Professional Activities, Grants and Awards

2001 2^{nd} place at the Bryansk region school Olympiad in physics.

2015-2016 Research Grant RFBR (Russian Foundation for Basic Research) №16-32-00157-mola. "Strongly correlated fermion systems within Density Functional Theory: quantum transport, ultra-cold atoms and solid state phenomena".

2016-present Peer Reviewer, The Journal of Chemical Physics.

Current Skills

During my master thesis research work I took first steps to the area of large-scale **DFT** calculations on supercomputers and also at that time I enhanced theoretical knowledge of DFT and its application to the solid state physics and the lattice dynamics calculations. Furthermore I gained large experience in computer science and numerical simulations, which includes operating systems, platforms, compilers and numerical methods. The work have been done in collaboration with JSCC RAS (Joint Supercomputer Center of the Russian Academy of Sciences) on the cluster MVS-15000BM by using MPICH programming environment.

During my PhD research I have written a computer code for **Time Dependent DFT** calculations for Hubbard Model in combination with **DMFT** calculations. The program consists of approximately 2000 lines in total with employment of efficient parallel and mathematical methods. I also developed a *xc* potential using numerical solution of 1D Bethe-Ansatz equation. The development of the code by using Shared Memory Programming With OpenMP have been done with close collaboration with two Swedish National Infrastructure for Computing meta-centers (SNICs): LUNARC (center for scientific and technical computing for research at Lund) and SNIC (Swedish National Supercomputer Center at Linköping).

During my PostDoc activity in CEA several modifications of the Quantum Espresso code were made in order to calculate the electron-vibration coupling for a molecules. Thereupon by use of model system based on the **Keldysh formalism** in combination with *ab initio* electron-vibron coupling results the picture of STM conductivity measurement was predicted.

Languages

Russian **Mother Tongue**, *Scientific Writing and Communication Skills.*

English **Fluently**, *Scientific Writing and Public Speaking Skills.*

Swedish **Elementary**.

French **Elementary**.

Computer Skills

Languages	Fortran, C, C++, HTML5, AWK, BASH, LaTeX
Protocols	OpenMP, MPI
Libraries	Lapack, BLAS, ScaLapack, Mkl, NAG
Sc. Packages	Maple, Matlab, Mathematica, Xmgrace, Gnuplot, **VASP, Quantum Espresso**
Other	Microsoft Office, OpenOffice, Adobe Acrobat
Platforms	Unix, Linux, Windows

Conference Proceedings

1 E.I. Isaev, Yu.Kh. Vekilov, A.I. Kartsev,*Ab-inito investigation of electronic and dynamical properties of heat-resistant materials*, Proc. of 61 scientific conference of students and young scientists of MISA (2006).

2 A.A. Artamonov, I.D. Bleskov, A.I. Kartsev, N.G. Bondarenko, E.I. Isaev, Yu.Kh. Vekilov, M.I, Katsnelson, *Lattice dynamics of B2 RuAl*, Proc. of the International Russian-Japan Symposium, 18-19 September, Saratov, Russia, pp. 843-849, 2007

3 Yu.Kh. Vekilov, E.I. Isaev, A.I. Kartsev, *Ab-inito investigation of electronic, magnetic and dynamical properties of iron mononitride*, Proc. of 62 scientific conference of students and young scientists of MISA (2007).

4 Yu.Kh. Vekilov, E.I. Isaev, A.I. Kartsev, $Ab-inito$ *investigation of lattice dynamic of new heat-resistant materials*, Proc. of 62 scientific conference of students and young scientists of MISA (2007).

6 A.I. Kartsev, E.I. Isaev, Yu.Kh. Vekilov, I.A. Abrikosov, B. Johansson, Magnetism of FeN from first principles, Moscow International Symposium on Magnetism, June 20-25, Moscow, Russia, p. 524, 2008.

7 A.I. Kartsev, Yu.Kh. Vekilov, E.I. Isaev, I.A. Abrikosov and B. Johansson, *Stability of the face-centered-cubic phases of CoN under pressure*, Fifth International Alloy Conference (IAC-V), september 11-14 2008, Ruegen, Germnay.

8 A.G. Beresnev, A.I. Kartsev, V.I. Razumovskiy, A.S. Trushnikova, *Effect of alloying elements and impurity (N) on bulk and grain boundary cohesion in Cr-base alloys*, The 7th International Conference on Computer Engineering and Technology (ICCET 2015), Paris, France.

9 A.I. Kartsev, N.G. Bondarenko, I.A. Abrikosov, *Magnetism and dynamic stability of Co, Fe and Cr mononitrides from first principle calculations*, International conference "Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures", 21-25 September 2015 Tomsk, Russia. `http://www.ispms.ru/files/Conference/2015/tezis_2015.pdf`

10 A. Kartsev, N. Bondarenko, *Thermodynamic properties of NiAs-FeN phase from first principles*, Proceedings of the 2015 International Conference on Simulation, Modelling and Mathematical Statistics(SMMS2015), November 22-23 2015, Chiang Mai, Thailand.

Publications

1 V. Vettchinkina, A. Kartsev, D. Karlsson, C. Verdozzi, *Interacting fermions in 1D disordered lattices: Exploring localization and transport properties with lattice density functional theories,* Phys. Rev. B 87, 115117 (2013). DOI: https://doi.org/10.1103/PhysRevB.87.115117

2 A. Kartsev, D. Karlsson, A. Privitera and C. Verdozz, *Three-dimensional dynamics of a fermionic Mott wedding-cake in clean and disordered optical lattices,* Scientific Reports 3, 2570 (2013) (Nature Publishing Group). DOI: 10.1038/srep02570

3 A. Kartsev, C. Verdozzi and G. Stefanucci, *Nonadiabatic Van der Pol oscillations in molecular transport,* The European Physical Journal B 87 (1), 1-12 (2014). DOI: 10.1140/epjb/e2013-40905-5

4 A. Kartsev, *Non-equilibrium fermions within lattice density functional theory: quantum transport and ultracold-atom phenomena.* Lund University, 2013. http://lup.lub.lu.se/search/record/3737651 ISBN: 978-91-7473-561-1

5 V.N. Butrim, I.M. Razumovskii, A.G. Beresnev, A. Kartsev, V.I. Razumovskiy, A.S. Trushnikova, *Effect of alloying elements and impurity (N) on bulk and grain boundary cohesion in Cr-base alloys,* Advanced Materials Research Volume 1119 (2015) pp 569-574. DOI: 10.4028/www.scientific.net/AMR.1119.569

6 A. Kartsev and N. Bondarenko, *Thermodynamic properties of NiAs-FeN phase from first principles*, proceedings of the 2015 International Conference on Simulation, Modelling and Mathematical Statistics (SMMS 2015) DEStech Publications, Inc. ISBN: 978-1-60595-112-6.

7 Boström, E., Hopjan, M., Kartsev, A., Verdozzi, C. and Almbladh, C.O., *Nonequilibrium Green's functions and atom-surface dynamics: Simple views from a simple model system.* Journal of Physics: Conference Series (Vol. 696, No. 1, p. 012007) 2016, March. IOP Publishing. DOI: 10.1088/1742-6596/696/1/012007

8 K. Bairagi, O. Iasco, A. Bellec, A. Katsev, J. Lagoute, C. Chacon, Y. Girard, S. Rousset, Y. Dappe, A. Smogunov, C. Barreteau, M. Boillot, T. Mallah, V. Repain, *Molecular-scale dynamics of light-induced spin cross-over in a two-dimensional layer*, 2016. Nature Communications 7, Article number: 12212. DOI: 10.1038/ncomms12212

9 A. Kartsev, N. Bondarenko, *Noval hexagonal FeN phase: high pressure stability and magnetism*, submitted to Journal of Applied Physics.

References

Professor Dr. Claudio Verdozzi.
Division of Mathematical Physics and
European Theoretical Spectroscopy Facility, Lund University.
Address: Division of Mathematical Physics, Department of Physics,
Lund University, Box 118, SE - 221 00 Lund, Sweden.
Phone: +46-46-2229499 E-mail: cv@teorfys.lu.se
http://www.matfys.lth.se/staff/Claudio.Verdozzi/

Professor Dr. Yuri Vekilov.
Department of Theoretical Physics and Quantum Technologies,
National University of Science and Technology «MISiS».
Address: MISiS, Leninskiy prospekt 4, 119049 Moscow, Russia.
Phone: +7-495-6384506 E-mail: yuri.vekilov@gmail.com
http://misis.ru/tpqt/staff/vekilov

Professor Dr. Cecilia Jarlskog.
Department of Mathematical Physics,
Lund Institute for Technology, Lund University, Sweden.
Phone: +46-46-222 3151 E-mail: cecilia.jarlskog@matfys.lth.se
Address: Division of Mathematical Physics, Department of Physics,
Lund University, Box 118, SE - 221 00 Lund, Sweden.
http://www.lunduniversity.lu.se/lucat/user/300c8a2e52261aff94132d5069d591c9

Dr. Daniel Karlsso.
Department of Physics, Nanoscience Center,
University of Jyvaškyla.
Phone: +358-40-805 4445 E-mail: daniel.l.e.karlsson@jyu.fi
Address: Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyvaškyla,
Finland.
https://www.jyu.fi/fysiikka/en/personnel/new/dalaerka

Research Geophysicist Dr. Antonio Privitera.
Geoscience company CGG.
Phone: +44 (0)1293683466 E-mail: antonioprivitera@gmail.com
Address: CGG Crompton Way, Manor Royal Estate,
Crawley, West Sussex RH10 9QN, United Kingdom.