Dmitry A. Ryndyk (Priv.-Doz. Dr. rer. nat. habil.) - Curriculum Vitae

Personal data

Date of birth: 02.04.1971
Family: married, 4 children
Address: Bremen Center for Computational Materials Science
Department of Physics
University of Bremen
Am Fallturm 1, 28359 Bremen, Germany
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Education

1994 Graduation (Diploma in Physics, with distinction), University of Nizhny Novgorod, Russia.
Diploma thesis: “Collective Josephson effect in superconducting micronetworks”.
2000 Ph.D. in Physics, Institute for Physics of Microstructures, Nizhny Novgorod, Russia.
Thesis: “Nonequilibrium effects in the dynamics of Josephson structures”.
2015 Habilitation in Physics, Institute for Theoretical Physics, University of Regensburg, Germany.
Thesis: “Modeling of quantum transport at the molecular scale”.

Scientific career / employment

Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod, Russia.
1994 – 1997 Junior Researcher.
1997 – 2001 Researcher.

Institute for Theoretical Physics, University of Regensburg, Germany.
2000 – 2001 Graduate College Fellow.
2002 – 2012 Researcher (Wissenschaftlicher Mitarbeiter).
from 2015 Privatdozent.

Institute for Materials Science, Technische Universität Dresden (TU Dresden), Germany.
2012 – 2017 Senior scientist and lecturer, research group leader (Nanoscale Modeling Group).

Bremen Center for Computational Materials Science, Department of Physics, Universität Bremen, Germany.
from 2016 Senior scientist and lecturer, research group leader.

Main results in research and teaching

More than 60 publications in the fields of theoretical physics, materials sciense, nano sciense.

D.A. Ryndyk,
Theory of Quantum Transport at Nanoscale (An introduction),
Springer, Series in Solid-State Sciences 184 (2016).

DFTB+XT: open software package for nanoscale modeling
http://quantranspro.org/dftb+xt

Teaching: 6 lecture courses in 4 universities, more than 10 exercise courses in theoretical physics.

Main expertise

Quantum transport, non-equilibrium effects and quantum many-body systems at nanoscale.

Theory and computational modeling of atomic and molecular nanostructures.

Other interests: nonequilibrium superconductivity, many-particle theory, strongly-correlated electron systems, Luttinger liquids, spin-liquids, high-T_C superconductors, plasma physics.

Present research interests – Theoretical and computational quantum transport

Quantum transport at nanoscale (dephasing and dissipation, strong nonequilibrium and many-body effects, time-dependent transport, *ab initio* atomistic approach).

Quantum materials (2D materials, surface chemistry & molecular electronics, topological states, calculation of material parameters from first principles, STM imaging and spectroscopy).

Nanoscale device modeling (molecular electronics, hybrid nanodevices, thermoelectric properties, nanocarbon based devices, 2D materials based devices).

Multiscale computational platform (multiscale and multiphysics approach linking atomistic *ab initio* description, quantum transport methods and 3D continuous methods, DFTB$^+$, CP2K, … software packages).

DFTB$^+$XT open software package for quantum nanoscale modeling.

Books

D.A. Ryndyk,
Theory of Quantum Transport at Nanoscale (An introduction),
Springer, Series in Solid-State Sciences 184 (2016).

Selected Publications

D.A. Ryndyk,
Collective dynamics of intrinsic Josephson junctions in high-T_c superconductors,
Phys. Rev. Lett. **80**, 3376 (1998).

E. Shapir, H. Cohen, A. Calzolari, C. Cavazzoni, D.A. Ryndyk, G. Cuniberti, A. Kotlyar, R. Di Felice, D. Porath,
Electronic structure of single DNA molecules resolved by transverse scanning tunnelling spectroscopy,
Nature Materials **7**, 68 (2008).

D.A. Ryndyk, M. Hartung, G. Cuniberti,
Nonequilibrium molecular vibrons: An approach based on the nonequilibrium Green function technique and the self-consistent Born approximation,
Phys. Rev. B **73**, 045420 (2006).

D.A. Ryndyk, A. Donarini, M. Grifoni, K. Richter,
Many-body localized molecular orbital approach to molecular transport,
Phys. Rev. B **88**, 085404 (2013).

D.A. Ryndyk, P. D'Amico, G. Cuniberti, K. Richter,
Charge-memory polaron effect in molecular junctions,
Phys. Rev. B **78**, 085409 (2008).

A. Franz, Y. Koval, D. Vasyukov, P. Müller, H. Schneidewind, D.A. Ryndyk, J. Keller, C. Helm,
Thermal fluctuations in ultrasmall intrinsic Josephson junctions,
Phys. Rev. B **69**, 014506 (2004).

S. Rother, Y. Koval, P. Müller, R. Kleiner, D.A. Ryndyk, J. Keller, C. Helm,
Charge-imbalance effects in intrinsic Josephson systems,
Phys. Rev. B **67**, 024510 (2003).

M. Fuechsle, J. Bentner, D.A. Ryndyk, M. Reinwald, W. Wegscheider, C. Strunk,
Effect of Microwaves on the Current-Phase Relation of Superconductor-Normal-Metal-Superconductor Josephson Junctions,
Phys. Rev. Lett. **102**, 127001 (2009).

D.A. Ryndyk, B. Song, R. Guttierrez, G. Cuniberti,
Green function techniques in the treatment of quantum transport at the molecular scale,
in *Energy Flow Dynamics in Biomaterial Systems*, eds. E. Bittner, V. May, D.A. Micha, and I. Burghardt, Springer series in Chemical Physics, page 213, Springer, Heidelberg, (2009).

Publications in referred journals

50 F. Eisenhut, T. Lehmann, A. Viertel, D. Skidin, J. Krüger, S. Nikipar, D. A. Ryndyk, C. Joachim, S. Hecht, F. Moresco, G. Cuniberti,
On-Surface Annulation Reaction Cascade for the Selective Synthesis of Diindenopyrene,
ACS Nano **11**, 12419 (2017).

49 J. Krüger, F. Eisenhut, T. Lehmann, J. M. Alonso, J. Meyer, D. Skidin, R. Ohmann, D. A. Ryndyk, D. Pérez, E. Guitián, D. Peña, F. Moresco, G. Cuniberti,
Molecular Self-Assembly Driven by On-Surface Reduction: Anthracene and Tetracene on Au (111),
J. Phys. Chem. C **121**, 20353 (2017).

48 J. Krüger, F. Eisenhut, J. M. Alonso, T. Lehmann, E. Guitián, D. Pérez, D. Skidin, F. Gamaleja, D. A. Ryndyk, C. Joachim, D. Peña, F. Moresco, G. Cuniberti,
Imaging the electronic structure of on-surface generated hexacene,
Chem. Comm. **53**, 1583 (2017).

47 M. Zwierzycki and D. A. Ryndyk,
Magnetic Properties of Hexagonal Graphene Nanomeshes,
Acta Physica Polonica A. **131** , 830 (2017).

46 A. Nickel, T. Lehmann, J. Meyer, F. Eisenhut, R. Ohmann, D.A. Ryndyk, C. Joachim, F. Moresco, G. Cuniberti,
Electronically Driven Single-Molecule Switch on Silicon Dangling Bonds,
J. Phys. Chem. C **120**, 27027 (2016)

45 A. Fediai, D.A. Ryndyk, G. Seifert, S. Mothes, M. Schröter, M. Claus, G. Cuniberti,
Impact of incomplete metal coverage on the electrical properties of metal-CNT contacts: large-scale *ab-initio* study,
Appl. Phys. Lett. **109**, 103101 (2016).

44 A. Fediai, D.A. Ryndyk, G. Cuniberti,
The modular approach enables a fully *ab initio* simulation of the contacts between 3D and 2D materials,
J. Phys.: Condens. Matter **28**, 395303 (2016).

43 J. Meyer, R. Ohmann, A. Nickel, C. Toher, R. Gresser, K. Leo, D.A. Ryndyk, F. Moresco, G. Cuniberti,
Influence of organic ligands on the line shape of the Kondo resonance,
Phys. Rev. B **93**, 155118 (2016).

42 A. Fediai, D.A. Ryndyk, G. Seifert, S. Mothes, M. Claus, M. Schröter, G. Cuniberti,
Towards an optimal contact metal for CNTFETs,
Nanoscale **8**, 10240 (2016).

41 A. Dianat, D.A. Ryndyk, G. Cuniberti,
Contact-dependent mechanical properties of graphene nanoribbons: An ab initio study,
Nanotechnology **27**, 025702 (2016).

40 T. Lehmann, D.A. Ryndyk, G. Cuniberti,
Thermoelectric properties of nanocarbons: atomistic modeling,
Physica Status Solidi A **213***,* 591 (2016).

39 T. Lehmann, D.A. Ryndyk, G. Cuniberti,
Enhanced thermoelectric figure of merit in polycrystalline carbon nanostructures,
Phys. Rev. B **92**, 035418 (2015).

38 A. Fediai, D.A. Ryndyk, G. Cuniberti,
Electron transport in extended carbon-nanotube/metal contacts: Ab initio based Green function method,
Phys. Rev. B **91**, 165404 (2015).

37 J. Meyer, A. Nickel, R. Ohmann, Lokamani, C. Toher, D.A. Ryndyk, Y. Garmshausen, S. Hecht, F. Moresco, G. Cuniberti,
Tuning the formation of discrete coordination nanostructures,
Chem. Commun. **51***,* 12621 (2015).

36 E. Baek, S. Pregl, M. Shaygan, L. Römhildt, W.M. Weber, T. Mikolajick, D.A. Ryndyk, L. Baraban, G. Cuniberti,
Optoelectronic Switching of Nanowire-based Hybrid Organic/Oxide/Semiconductor Field-Effect Transistors,
Nano Research **8**, 1229 (2015).

35 H. Sevincli, T. Lehmann, D.A. Ryndyk, G. Cuniberti,
Comparison of electron and phonon transport in disordered semiconductor carbon nanotubes,
Journal of Computational Electronics ***12***, 685 (2013).

34 M. Hinreiner, D.A. Ryndyk, D. Usvyat, T. Merz, M. Schütz, K. Richter,
Influencing the conductance in biphenyl-like molecular junctions with THz radiation,
Physica Status Solidi (b) **250**, 2408 (2013).

33 T. Lehmann, D.A. Ryndyk, G. Cuniberti,
Combined effect of strain and defects on the conductance of graphene nanoribbons,
Phys. Rev. B **88**, 125420 (2013).

32 D.A. Ryndyk, A. Donarini, M. Grifoni, K. Richter,
Many-body localized molecular orbital approach to molecular transport,
Phys. Rev. B **88**, 085404 (2013).

31 D.A. Ryndyk, J. Bundesmann, M.H. Liu, K. Richter,
Edge state effects in junctions with graphene electrodes,
Phys. Rev. B **86**, 195425 (2012).

30 N. Grib, D.A. Ryndyk, R. Guttierrez, G. Cuniberti,
Distance-dependent coherent charge transport in DNA: crossover from tunneling to free propagation,
Journal of Biophysical Chemistry **1**, 77 (2010).

29 D.A. Ryndyk, P. D'Amico, K. Richter,
Single-spin polaron memory effect,
Phys. Rev. B **81**, 115333 (2010), arXiv:0904.3839.

28 D.A. Ryndyk, E. Shapir, D. Porath, A. Calzolari, R. Di Felice, G. Cuniberti,
Scanning tunnelling spectroscopy of single DNA molecules,
ACS Nano **3**, 1651 (2009).

27 M. Fuechsle, J. Bentner, D.A. Ryndyk, M. Reinwald, W. Wegscheider, C. Strunk,
Effect of Microwaves on the Current-Phase Relation of Superconductor-Normal-Metal-Superconductor Josephson Junctions,
Phys. Rev. Lett. **102**, 127001 (2009), arXiv:0707.4512.

26 E. Pallecchi, M. Gaass, D.A. Ryndyk, C. Strunk,
Carbon nanotube Josephson junctions with Nb contacts,
Appl. Phys.Lett **93**, 072501 (2008), arXiv:0804.0168.

25 P. D'Amico, D.A. Ryndyk, G. Cuniberti, K. Richter,
Charge-memory effect in a polaron model: equation-of-motion method for Green functions,
New J. Phys. **10**, 085002 (2008), arXiv:0806.1633

24 D.A. Ryndyk, P. D'Amico, G. Cuniberti, K. Richter,
Charge-memory polaron effect in molecular junctions,
Phys. Rev. B **78**, 085409 (2008), arXiv:0802.2808.

23 E. Shapir, H. Cohen, A. Calzolari, C. Cavazzoni, D.A. Ryndyk, G. Cuniberti, A. Kotlyar, R. Di Felice, and D. Porath,
Electronic structure of single DNA molecules resolved by transverse scanning tunnelling spectroscopy,
Nature Materials **7**, 68 (2008).

22 D.A. Ryndyk and G. Cuniberti,
Nonequilibrium resonant spectroscopy of molecular vibrons,
Phys. Rev. B **76**, 155430 (2007), cond-mat/0701086.

21 Bo Song, D.A. Ryndyk, G. Cuniberti,
Molecular junctions in the Coulomb blockade regime: rectification and nesting,
Phys. Rev. B **76**, 045408 (2007), cond-mat/0611190.

20 D.A. Ryndyk, M. Hartung, G. Cuniberti,
Nonequilibrium molecular vibrons: An approach based on the nonequilibrium Green function technique and the self-consistent Born approximation,
Phys. Rev. B **73**, 045420 (2006).

19 D.A. Ryndyk and J. Keller,
Inelastic resonant tunneling through single molecules and quantum dots: spectrum modification due to nonequilibrium effects,
Phys. Rev. B **71**, 073305 (2005).

18 J. Keller and D.A. Ryndyk,
Static charge-imbalance effects in intrinsic Josephson systems,
Phys. Rev. B **71**, 054507 (2005).

17 Ch. Helm, L.N. Bulaevskii, D.A. Ryndyk, J. Keller, S. Rother, Y. Koval, P. Müller, R. Kleiner,
Electronic compressibility and charge imbalance relaxation in cuprate superconductors,
Physica C **408**, 612 (2004).

16 V.V. Khodos, D.A. Ryndyk, V.L.Vaks,
Fast-passage microwave molecular spectroscopy with frequency sweeping,
EPJ Appl. Phys. **25**, 203 (2004).

15 A. Franz, Y. Koval, D. Vasyukov, P. Müller, H. Schneidewind, D.A. Ryndyk, J. Keller, C. Helm,
Thermal fluctuations in ultrasmall intrinsic Josephson junctions,
Phys. Rev. B **69**, 014506 (2004).

14 D.A. Ryndyk, N. V. Demarina, J. Keller, E. Schomburg,
Superlattice with hot electron injection: An approach to a Bloch oscillator,
Phys. Rev. B **67**, 033305 (2003).

13 S. Rother, Y. Koval, P. Müller, R. Kleiner, D.A. Ryndyk, J. Keller, C. Helm,
Charge-imbalance effects in intrinsic Josephson systems,
Phys. Rev. B **67**, 024510 (2003).

12 D.A. Ryndyk, J. Keller, C. Helm,
Non-equilibrium effects due to charge fluctuations in intrinsic Josephson systems,
J. Phys.: Cond. Mat. **14**, 815 (2002).

11 E.V Suvorov and D.A. Ryndyk,
Stochastic broadening of ion cyclotron resonances due to development of lower hybrid turbulence,
Phys. Lett. A **282**, 31 (2001).

10 D.A. Ryndyk, V.I. Pozdnjakova, I.A. Shereshevskii, N.K. Vdovicheva,
Dynamics and transformations of the Josephson vortex lattice in layered superconductors,
Phys. Rev. B **64**, 052508 (2001).

9 D.A. Ryndyk,
High-frequency properties of nonequilibrium Josephson junctions in submicron superconductors,
Advances of radioelectronics [*Uspekhi radioelektroniki,* in russian], n. 2, p. 53 (2001).

8 D.A. Ryndyk,
Nonequilibrium Josephson effect in systems of tunnel superconducting junctions and in layered superconductors,
JETP **89**, 975 (1999) [Zh. Eksp. Teor. Fiz. **116**, 1798 (1999) in russian].

7 D.A. Ryndyk,
Collective dynamics of intrinsic Josephson junctions in high-T_c superconductors,
Phys. Rev. Lett. **80**, 3376 (1998).

6 E.V. Suvorov, D.A. Ryndyk et al.,
Low-hybrid turbulence excited by transverse ion beam in a magnetized plasma,
Nuclear Fusion **38**, 661 (1998).

5 E.V. Suvorov, D.A. Ryndyk et al.,
Collective Thomson scattering at W7-AS,
Plasma Phys. & Contr. Fussion **39B**, 337 (1997).

4 D.A. Ryndyk,
Quasiparticle dynamics and phase locking in a S-I-S multilayer Josephson junction,
JETP Lett. **65**, 791 (1997).

3 A.P. Protogenov and D.A. Ryndyk,
Marginal Fermi liquid in strongly correlated spin systems,
Modern Physics Letters **8**, 859 (1994) .

2 D.A. Ryndyk,
Fluctuation-dynamic instability and induced resistive state in long Josephson junction,
Radiophysics and Quantum Electronics **36**, 543 (1993).

1 V.V. Kurin and D.A. Ryndyk,
Coherent microwave – induced effects in 2D Josephson arrays,
Physica C **205**, 85 (1993).

Book chapters

A4 D.A. Ryndyk, B. Song, R. Guttierrez, G. Cuniberti,
Green function techniques in the treatment of quantum transport at the molecular scale,
in *Energy Flow Dynamics in Biomaterial Systems*, eds. E. Bittner, V. May, D.A. Micha, and I. Burghardt, Springer series in Chemical Physics, page 213, Springer, Heidelberg, (2009), arXiv:0805.0628.

A3 E.V. Suvorov and D.A. Ryndyk,
Stochastic Broadening of High Order Ion Cyclotron Resonances due to LH Turbulence,
in *Strong microwaves in plasmas II*, ed. A.G. Litvak, Nizhny Novgorod (2000).

A2 E.V. Suvorov, D.A. Ryndyk et al.,
Low-hybrid turbulence excited by transverse ion beam in a magnetized plasma,
in *Strong microwaves in plasmas*, ed. A.G. Litvak, v. 2, p. 468, Nizhny Novgorod, Russia (1997).

A1 E.V. Suvorov, D.A. Ryndyk et al.,
Experiments on the collective Thomson scattering of powerful 140 GHz radiation at W7-AS,
in *Strong microwaves in plasmas* , ed. A.G. Litvak, v. 1, p. 129, Nizhny Novgorod, Russia (1997).

Selected Conference Proceedings

P10 M. Claus, A. Fediai, S. Mothes, J. Knoch, D.A. Ryndyk, S. Blawid, G. Cuniberti, M. Schröter,
Towards a multiscale modeling framework for metal-CNT interfaces,
2014 International Workshop on Computational Electronics (IWCE), p. 1 (2014).

P9 A. Fediai, D.A. Ryndyk, G. Cuniberti,
Contact properties of ultrasmall carbon nanotube transistors from Ab-initio,
EEE 34th International Conference on Electronics and Nanotechnology (ELNANO), p. 110 (2014).

P8 E.V. Suvorov, D.A. Ryndyk et al.,
Collective scattering of powerful 140 GHz radiation at W7-AS,
Europhysics conference abstracts **19C-I**, 429 (1995).

P7 A.A. Andronov, V.V. Kurin, M.Yu. Levichev, D.A. Ryndyk, V.I. Vostokov,
Fluxoid logic,
Proceedings of 6 Trilateral Germ.-Russ.-Ukr. Seminar on HTSC, p. 158, Dubna, Russia (1994).

P6 A.A. Andronov, V.V. Kurin, M.Yu. Levichev, D.A. Ryndyk, V.I. Vostokov,
Superconductor fluxoid logic,
in *Applied superconductivity (proceedings of the European Conference on Applied Superconductivity)*, ed. H.C. Freyhardt, p. 1469, Göttingen, Germany (1993).

P5 A.A. Andronov, V.V. Kurin, M.Yu. Levichev, D.A. Ryndyk, V.I. Vostokov,
Fluxoid logic based on frustrated Josephson arrays,
Proceedings of the International Superconductive Electronics Conference (ISEC'93), p. 60, Boulder, U.S.A. (1993).

P4 A.P. Protogenov and D.A. Ryndyk,
Microscopic origin of marginal Fermi-liquid in strongly correlated spin system,
*J. Appl. Phys.***73**, 6651 (1993).

P3 V.V. Kurin, D.A. Ryndyk, V.I. Vostokov,
Microwave induced effects in 2D arrays of Low-T_c Josephson junctions and High-T_c weak links,
Proceedings of the 5 German-CIS Seminar on HTSC, p. 66, Kloster Banz, Germany (1992).

P2 A.P. Protogenov and D.A. Ryndyk,
Microscopic origin of marginal Fermi-liquid in strongly correlated spin system,
ICTP preprint IC/92/211, Trieste, Italy (1992).

P1 D.A. Ryndyk,
Breather dynamics in an ac-driven long Josephson junction,
Proceedings of the School-seminar on Dynamic and Stochastic Wave Phenomena, p. 115, Nizhny Novgorod, Russia (1992).

Teaching

Lecture Courses (2 hours per week)

1999 - *Superconductivity* at the University of Nizhny Novgorod.
1999/2000 - *Classical Mechanics* at the University of Nizhny Novgorod.
2004/05 - *Quantum Transport in Nanostructures* at the University of Regensburg.
2006/07 - *Theory of Quantum Transport through Nanosystems* at the University of Regensburg.
2011/12 - *Advanced theory of quantum transport in nanosystems* at the University of Regensburg.
2012 - *Introduction to the theory of molecular transport at nanoscale* at the University of Regensburg.
2012/13 - *Primer of quantum transport at nanoscale* at the Technische Universität Dresden.
2014 - *Nanostructured Materials* at the Technische Universität Dresden.
2015 - *Nanostructured Materials* at the Technische Universität Dresden.
2016 - *Nanostructured Materials* at the Technische Universität Dresden.
2018 - *Theoretical and Computational Quantum Transport* at the Universität Bremen.

Tutorials

1995/96 - *Mathematical Physics* at the University of Nizhny Novgorod.
1996/97 - *Statistical Physics* at the University of Nizhny Novgorod.
1997/98 - *Quantum Mechanics* at the University of Nizhny Novgorod.
1998/99 - *Classical Mechanics* at the University of Nizhny Novgorod.
2002 - *Quantum Physics (Physik III: Wellen und Quanten)* at the University of Regensburg.
2003/04 - *Electrodynamics (Theoretische Physik II: Elektrodynamik)* at the University of Regensburg.
2004 - *Quantum Mechanics (Theoretische Physik III: Quantenmechanik)* at the University of Regensburg.
2004 - *Quantum Mechanics with Maple (Quantenmechanik mit Maple)* at the University of Regensburg.
2004/05 - *Mechanics (Physik I: Mechanik)* at the University of Regensburg.
2005 - *Classical Mechanics (Theoretische Physik I: Klassische Mechanik)* at the University of Regensburg.
2005/06 - *Mechanics (Physik I: Mechanik und Nichtlineare Dynamik)* at the University of Regensburg.
2008/09 - *Electrodynamics (Theoretische Physik II: Elektrodynamik)* at the University of Regensburg.
2009/10 - *Electrodynamics (Theoretische Physik Ib: Elektrodynamik)* at the University of Regensburg.
2010/11 - *Mesoscopic physics (Quantentheorie der kondensierten Materie II)* University of Regensburg.
2012/13 - *Molecular Modeling* at the Technische Universität Dresden.

Supervision of PhD, Diploma, Master

- B. Rieder, Ph.D., *Semiclassical transport in semiconductor superlattices with boundaries*, 2004.
- M. Hartung, diploma, *Vibrationseffecte im Ladungstransport durch molekulare Brücken*, 2004.
- P. D'Amico, Ph.D., *Switching and memory effects in electron-vibron systems*, 2010.
- M. Hinreiner, diploma, *Conformational effects on quantum transport through biphenyl-like junctions,* 2012.
- T. Lehmann, diploma, *Ab-initio and transport models for GNRs under mechanical stress and defects,* 2013.
- Y. Yang, master thesis, *Molecular Switches on Semiconductor Surfaces*, 2014.
- V. Gupta, master thesis, *Inelastic Dephasing and Dissipation for Atomistic Electron Transport,* 2016.
- T. Lehmann, Ph.D., present time.
- S. Nikipar, Ph.D., present time.
- P. Karrasch, Ph.D., present time.

Some last invited talks

1 Vielberth Symposium “DNA nanoelectronics: theory and experiment”,
Nonequilibrium quantum transport through DNA-like molecules,
Regensburg, Germany, April 2006.

2 Workshop “Shrovetide-nano-day”,
Nonequilibrium STM spectroscopy of single molecules,
Dresden, Germany, Februar 2007.

3 “The Nanophysics and Nanoelectronics Symposium”,
STM spectroscopy of single molecules: from simple complexes to DNA,
Nizhny Novgorod, Russia, March 2007.

4 Workshop “Modeling DNA charge migration”,
STM spectroscopy of single DNA molecules,
Regensburg, Germany, May 2007.

5 Workshop “Nonequilibrium Nanostructures”,
Nonequilibrium vibrons and polarons,
Dresden, Germany, December 2008.

6 Workshop “Quantum transport on the molecular scale”,
Modelling electronic transport through single molecules: vibrons and polarons,
Bremen, Germany, September 2009.

7 Workshop “Quantum transport in nanoscale molecular systems”,
Many-body localized molecular orbital approach to molecular transport ,
Telluride, U.S.A., August 2011.

8 Workshop “Molecular scale and organic electronic materials”,
Edge State Effects in Molecular Junctions with Graphene Electrodes,
Dresden, Germany, December 2012.

9 TUG/KFU Physics Colloquium, TU Graz
Charge transport at the molecular scale: is theory really predictive?,
Graz, Austria, January 2013.

10 Workshop “Molecular electronics: Quo vadis?”,
Many-body localized molecular orbital approach to molecular transport,
Bremen, Germany, March 2013.

11 Workshop “Novel Approaches to DNA Sequencing",
DNA Translocation through Graphene Nanopores and the Sequencing Problem: A Theoretical Study,
Stockholm, Sweden, Juni 2013.

12 School on Functional Nanomaterials,
Nanoscale thermoelectrics,
Dresden, Germany, October 2013.

13 CECAM Workshop “High performance models for charge transport in large scale materials systems”,
Modeling of quantum transport at nanoscale: localized molecular orbitals and vibrons,
Bremen, Germany, October 2014.

14 Physics Colloquium, Uni Regensburg
Complex nanoscale modeling: quantum transport in molecular electronics,
Regensburg, Germany, April 2015.

15 NanoNet Workshop
Modeling of molecular nanostructures on metal and semiconductor surfaces,
Dresden, Germany, September 2015.

16 Workshop on simulations of thermoelectric materials
Quantum charge and thermal transport at nanoscale: thermoelectric effects,
Rossendorf, Germany, February 2016.

17 Kick-Off Workshop of QM3 Research Training Group
Introduction to theoretical and computational quantum transport,
Bremen, Germany, March 2017.

18 TNT 2017 conference (Trends in Nanotechnology)
Atomistic nanoscale device modeling: charge and heat transport in large-scale systems,
Dresden, Germany, June 2017.

Brief description of the scientific achievements till 2012

Quantum transport theory at nanoscale and molecular electronics. The main field of research from 2000. Was started at the University of Regensburg in the group of Prof. J. Keller. Some investigations devoted to the nonequilibrium theory of semiconductor superlattices were performed in collaboration with the experimental group of Prof. K.F. Renk. In the paper [14] a new approach to a Bloch oscillator was considered.

From 2005 this work was continued in the junior research group "Molecular Computing" of Dr. G. Cuniberti and from 2007 in the group of Prof. K. Richter at the University of Regensburg. The main fields of research were nonequilibrium quantum transport through quantum dots and single molecules, Coulomb blockade in molecules, electron-vibron interaction, nonequilibrium STM spectroscopy of single molecules, transport in bio-molecules (DNA), and other related topics. The following results were obtained during this period. The approach based on the nonequilibrium Green function method and Keldysh technique was developed to describe finite-voltage transport through electron-vibron systems, in the paper [19] the spectrum modification effect was considered, in the paper [20] the general quantum theory of nonequilibrium vibrons and vibronic instability was formulated, and new features in the voltage-current curves were discussed. In the paper [22] the theory was applied to describe the vibronic features in the experiments in molecular junctions and STM-to-molecule junctions. The other approach, namely nonequilibrium equation-of-motion method, alternative to the Keldysh-Dyson method, was suggested [21] to describe the Coulomb blockade in multi-level systems. In particular, we considered the rectification effect in the Coulomb blockade regime. These theoretical results are related directly to recent experiments with single molecules. The other results are devoted to the experiments on electron transport in DNA [23,28,30]. Finally, in the papers [24,25,29] charge and spin polaron memory effects are considered.

The results of some of these investigations are summarized in the review [A4].

Nonequilibrium Superconductivity and Josephson effect. Student research was devoted to different aspects of the theory of superconductors, including the dynamics of long Josephson junctions [P1,2], the theory of high-T_C superconductivity in strongly correlated electron systems [P2,P4,3], microwave induced effects in Josephson arrays [P3,1], fluxoid logic and memory [P5,P6,P7]. This work was done in collaboration and under supervision of Prof. A.A. Andronov, Prof. V.V. Kurin, and Prof. A.P Protogenov. These results were reviewed in the diploma thesis.

Ph.D. research project was devoted to nonequilibrium effects in the dynamics of Josephson structures. The investigation was initially devoted to the quasiparticle (charge-imbalance) coupling mechanism between Josephson junctions [4]. Later, besides the systems of tunnel junctions, intrinsic Josephson junctions in high-temperature superconductors become the main subject of research. Macroscopic [7] and microscopic [8] theories were developed. Some high-frequency properties of nonequilibrium Josephson junctions were considered in [9,10]. The intermediate results were summarized in the Ph.D. thesis (2000). The work in this direction was continued together with Prof. J. Keller at the University of Regensburg. A comprehensive theory of charge-imbalance effects in intrinsic Josephson systems was developed [12,13,17,18]. The effective collaboration with the experimental groups of Prof. P. Müller (Uni Erlangen) and Prof. R. Kleiner (Uni Tübingen) resulted in the paper [13] devoted to the charge-imbalance experiments, and the paper [15], where the thermal fluctuations of ultra-small intrinsic Josephson junctions were investigated experimentally and theoretically. The work in the field of nonequilibrium Josephson effect in mesoscopic S-N-S structures is continued also in the University of Regensburg in collaboration with Prof. Ch. Strunk [26,27].

Plasma physics, theory of plasma instabilities. This work, being continued for several years, was a result of the cooperation between the plasma physics department of the Applied Physics Institute in Nizhny Novgorod, Russia and the team of the W7-AS stellarator in Garching, Germany. The theory of ion beam induced low-hybrid instabilities in hot plasma was developed to explain the results of experiments on the collective scattering of microwave radiation [P8,A1,A2,A3,5,6,11]. The theoretical calculations in these papers were performed together with E.V. Suvorov.

Nanoscale Modeling Group 2012-2017

The focus topic of the Nanoscale Modeling Group at the Chair Materials Science and Nanotechnology of Prof. G. Cuniberti, Institute for Materials Science, TU Dresden is development and application of semi-empirical and *ab initio* based quantum transport methods to describe nonequilibrium phenomena in molecular nanosystems and nanomaterials. Recent and current topics include: *Ab initio* modeling of molecular junctions with semiconductor electrodes; Thermoelectric effects in nanocarbons, hybrid materials and molecular junctions [35,39,40]; Quantum theory of phonon (vibron) thermal flow in molecular junctions [35,39]; *Ab initio* modeling of organic molecules on metal and semiconductor surfaces [37,43,47,48,49,50]; Kondo effect in strongly asymmetric molecular junctions [43]; DNA sequencing in graphene nanopores; Many-body and time-dependent theory of molecular transport [32,34]; Graphene electrodes for molecular electronics [31]; Plane molecular electronics; Molecular switches [46] and logic circuits; Metal/nanocarbon contacts and CNT-FETs [P9,P10,38,41,42,44,45]; Stress and defects in nanocarbons [33,35,41]; Hybrid molecular/semiconductor devices [36,39].

In particular

- An *ab initio* based theoretical approach to describe nonequilibrium many-body effects in molecular transport is developed. We introduce a basis of localized molecular orbitals and formulate the many-body model in this basis. In particular, the Hubbard-Anderson Hamiltonian is derived for single-molecule junctions with intermediate coupling to the leads [32]. This approach can be also used as a basis for transport theory in large-scale systems and for molecules on surfaces.
- The combined influence of structural defects and uniaxial longitudinal strain on the electronic transport properties of armchair graphene nanoribbons was investigated using the numerical approach based on the semiempirical tight-binding model, the Landauer formalism, and the recursion method for Green functions [33]. The conductance of graphene nanoribbons was calculated in the quantum coherent regime with different types and concentrations of defects, namely randomly distributed and oriented single and double vacancies and Stone-Wales defects.
- New computational method is developed and used to predict the electrical properties of contacts in realistic carbon nanotube field effect transistors (CNT-FETs) [38]. It is based on large-scale *ab initio* calculations combined with the Green function approach. For the first time, both internal and external parts of a realistic CNT-metal contact are taken into account at the *ab initio* level. Within the method, it is possible to calculate the transmission coefficient through a contact of both finite and infinite length; the local density of states can be determined in both free and embedded CNT segments. Perfect agreement with the experimental data for Pd and Al contacts is found.
- Using a combined approach of density functional theory and nonequilibrium Green functions the electron and phonon transport in carbon-based systems was investigated [39,40]. Quantum transport and thermoelectric properties are summarized for graphene sheets, graphene nanoribbons, and carbon nanotubes with a variety of defects and grain boundary types in a wide temperature range.

Finally, during this time the book “Theory of quantum transport at nanoscale” was finished and published.

Last projects/grants

At present time NanoMod group participates in the following German and European research programs:

2012 – 2016 DFG Priority Program SPP1386 “Nanostructured thermoelectrics”,
2012 – 2016 SMWK grant “Stress and defects in graphene”,
2012 – 2017 Int. Max Planck Res. School "Dynamical Processes in Atoms, Molecules and Solids",
2013 – 2017 Cluster of Excellence “Center for Advancing Electronics Dresden” (cfaed),
2013 – 2017 EU FP7 Project “Planar atomic and molecular scale devices” (PAMS),
2013 – 2017 EU FP7 Project “Nanocarbons for versatile power supply modules” (NanoCaTe),
2014 – 2017 Project “Graphene-based nanostructures for spintronics and spin caloritronics” (Harmonia),
2015 – 2018 International Helmholtz Research School “NanoNet”.