

Grigory Kolesov

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Education

- **M.S.** in Molecular Genetics, Novosibirsk State University, 1998
- 1999-2003: Graduate student at MIPS, Institute for Bioinformatics (IBI), German National Center for Health and Environment;
- **Ph.D.** in computational biology, Technical University of Munich, 2005
- 2009-2013: graduate student at the department of Physics and Astronomy, University of Wyoming
- **Ph.D.** in physics, University of Wyoming, 2013

Research experience

- 2004-2007: Postdoctoral fellow at Harvard-MIT Division of Health Sciences and Technology
- 2007-2009: Postdoctoral fellow at the University of Wyoming
- Summer 2012: Research internship at the Los Alamos National Laboratory
- 2013-now: Postdoctoral fellow at School of Engineering and Applied Sciences, Harvard University

Research interests

- Excited state dynamics, computational material science
- Condensed matter, nonequilibrium many-body physics, quantum chemistry
- Molecular dynamics
- Biophysics
- Electrochemistry
- Protein structure and function prediction
- Bioinformatics, genomics; evolution and phylogenetics, evolution of gene order

Teaching experience

- 2002 Technical University of Munich
Taught hands-on computational course on evolution and phylogenetics
- 2009 University of Wyoming
Teaching Assistant, general physics I, labs and discussions
Teaching Assistant, general physics II, labs and discussions
- 2015 Harvard University. Co-taught course “Computational Material Design”

Computational skills

- *Numerical methods and simulations; finite difference, spectral and Monte Carlo methods*
- *C/C++, FORTRAN, Perl, Python, Java, Haskell, Modula-2, Pascal, Matlab, Assembly (x86, Alpha)*
- *Quantum chemistry and solid state packages: Gaussian/ONIOM, QuantumEspresso, SIESTA, VASP, Abinit, YAMBO, ASE, ATAT (Alloy-Theoretic Automated Toolkit)*
- *bioinformatics tools: structural bioinformatics, Bioperl, Bioconductor, alignments and phylogeny/evolution tools*
- *Parallel programming, multi-threading, MPI, SCALAPACK, distributed computing, GPU programming (CUDA)*
- *Linux/UNIX/POSIX - application/system-level programming, administration, clusters, Kerberos/AFS administration and programming*
- *HPC, batch systems administration - LSF, Sun grid engine*
- *databases, SQL*
- *web programming, UI programming in Java*

Selected scientific software

- *TDAP2, Non-adiabatic excited state molecular dynamics with real time time-dependent density functional theory (TDDFT) based on SIESTA*
- *2TSE - Quantum kinetics; Kadanoff-Baym equation solver in two-time Chebyshev polynomials (applied to quantum dot sensitized solar cell).*
- *Non-adiabatic excited states molecular dynamics (LANL, 2012)*
- *elarraysim - electrochemistry diffusion and chemical step simulator for interdigitated ultramicroelectrode arrays*
- *Knot server - online prediction of knots in 3D-structures of proteins. (<http://knots.mit.edu>).*
- *msamc - Monte Carlo algorithm to assess the quality of*

- predicted specificity determining and co-evolving residues
- *pSDRdb* - database of automatically predicted specificity determining residues of bacterial protein domains. Online prediction of SDRs and correlated mutations.
 - *SNAPper* - Prediction of gene function based on gene order in prokaryotes using Similarity-Neighborhood Approach. Multithreaded distributed UNIX daemon and web interface.
 - *SNiPPER* - SNP-mining program.
 - Jaba - contig/genome-level annotation tool, used in Arabidopsis Thaliana and Neurospora crassa genome projects.

Conference Talks

1. Kolesov, G., Grånäs, O., Hoyt, R., Kaxiras, E. Time-dependent density functional theory and non-adiabatic Ehrenfest dynamics with localized basis sets: method and applications. *ES2015 Electronic Structure workshop*, 2015
2. Kolesov, G., Vinichenko, D., Tritsarlis, G. A., Friend, C. M., Kaxiras, E. Polarons in rutile TiO₂ surfaces: a non-adiabatic excited-state dynamics study. *APS March Meeting*, 2015
3. Kolesov, G., Vinichenko, D., Tritsarlis, G. A., Friend, C. M., Kaxiras, E. Non-Adiabatic Excited-State Dynamics Study of Methoxy photo-Oxidation on TiO₂₍₁₁₀₎ Surface, *Material Research Society (MRS) Fall Meeting*, 2014
4. Kolesov, G., Vinichenko, D., Tritsarlis, G., Friend, C., Kaxiras, E. Methoxy photo-oxidation on rutile TiO₂ surface : excited-state non-adiabatic dynamics study , *Dynamics Interactions and Electronic Transitions at surfaces (DIET) meeting*, 2014
5. Kolesov, G., Thermodynamic properties and band structure of zinc stannate Zn₂SnO₄ , *APS March Meeting*, 2014
6. Kolesov, G., and Dahnovsky, Y., Correlated electron transfer and nonlinear optical effects in QD sensitized solar cells, *APS April Meeting*, 2013, **58**, 4.
7. Kolesov, G., and Dahnovsky, Y., Nonequilibrium Green's function calculations in quantum dot sensitized solar cells: uncorrelated quantum dot electrons, *ACS National Meeting*, 2011

Publications

1. Kolesov, G., Grånäs, O., Hoyt, R., Kaxiras, E., Time-dependent density functional theory and non-adiabatic dynamics for a thousand of atoms: method and applications , *in preparation*
2. **Kolesov, G., Vinichenko, D., Tritsarlis, G. A., Friend, C. M., Kaxiras, E. Anatomy of the Photochemical Reaction: Excited-State Dynamics Reveals the C-H Acidity Mechanism of Methoxy Photo-oxidation on Titania , *JPC Letters*, 2015**
3. Tritsarlis, G. A., Vinichenko, D., Kolesov, G., Friend, C. M., Kaxiras, E. Dynamics of the Photogenerated Hole at the Rutile TiO₂₍₁₁₀₎/Water Interface: A Nonadiabatic Simulation Study, *JPC*, 2014
4. Liu, F., Kolesov, G., Parkinson, B.A. Preparation, Applications, and Digital Simulation of Carbon Interdigitated Array Electrodes , 2014, *Analytical Chemistry*

5. Liu, F., Kolesov, G., Parkinson, B.A. Time of Flight Electrochemistry: Diffusion Coefficient Measurements Using Interdigitated Array (IDA) Electrodes, 2014, Journal of The Electrochemical Society
6. Nepomnyashchii, A.B., Kolesov, G. and Parkinson, B.A. Electrogenerated Chemiluminescence of BODIPY, Ru(bpy)₃²⁺ and 9,10-Diphenylanthracene using Interdigitated Array Electrodes, 2013, ACS Applied Materials & Interfaces
7. Pimachev, A., Kolesov, G., Chen, J., Wang, W., and Dahnovsky, Y., Internal relaxation in dye sensitized solar cells based on Zn₂SnO₄ nanostructures, 2012, JCP
8. **Kolesov, G., Dahnovsky, Y., Correlated electron dynamics in quantum-dot sensitized solar cell: Kadanoff-Baym vs. Markovian approach, Phys. Rev. B, 2012; 85, 241309.**
9. Kolesov, G., Dahnovsky, Y., Quantum correlation effects in electron dynamics in molecular wires and solar cells: the nonequilibrium Green's function approach, Advances in Quantum Chemistry, Book Chapter, 2011; 61:261–315
10. Liberles, D., Kolesov, G., Dittmar, K., Understanding gene duplication through biochemistry and population genetics, Evolution After Gene Duplication, Book Chapter, Hoboken (NJ): Wiley-Blackwell, 2010
11. Kolesov, G., Mirny, L.A. Using evolutionary information to find specificity determining and co-evolving residues (2009), Computational Systems Biology, Book Chapter, Methods Mol Biol, Humana press, 2009;541:421-48.
12. Huzurbazar S, Kolesov G, Massey SE, Harris KC, Churbanov A, Liberles DA. Lineage-Specific Differences in the Amino Acid Substitution Process. J Mol Biol. 2010 Mar 12;396(5):1410-1421. Epub 2010 Jan 15.
13. Tellgren-Roth A, Kolesov G, Sifuentes-Rincón AM, Liberles DA. Complex microsatellite dynamics in the myostatin gene within ruminants (2008). J. Mol. Evol. 2008 Mar;66(3):258-65.
14. **Kolesov, G., Wunderlich, Z., Laikova, O.N., Gelfand, M.S., Mirny, L.A., How gene order is influenced by the biophysics of transcription regulation (2007), Proc Natl Acad Sci USA. 2007 Aug 28;104(35):13948-53.**
15. Kolesov, G., Virnau, P., Kardar, M., Mirny, L.A. (2007) Protein Knot Server: detection of knots in protein structures, Nucl Acids Res, 2007 May 21;
16. Kolker, E., Makarova, K., Shabalina, S., Picone, A., Purvine, S., Holtzman, T., Cherny, T., Ambruster, D., Munson, R., Kolesov, G., Frishman, D., Galperin, M. (2004). Identification and Functional Analysis of Conserved Hypothetical Genes Expressed in Hemophilus influenzae, Nucl Acids Res, 32(8):2353-61
17. Kota, R., Rudd S., Facius A., Kolesov G., Thiel T., Zhang H., Stein N., Mayer K., Graner A. (2003). SNipPing polymorphisms from the large barley EST collections. Molecular Genetics and Genomics, 270, 24-33
18. Wong, P., Kolesov, G., Frishman, D. Houry, W. (2003). Phylogenetic Web Profiler. Bioinformatics, Apr;19(6): 782-3.
19. Frishman, D., Mokrejs M., Kosykh D., Kastenmueller G., Kolesov G., Zubrzycki I., Gruber C., Geier B., Kaps A., Albermann K., Volz A., Wagner C., Fellenberg M., Heumann K., Mewes, H.-W. (2003). The PEDANT genome database. Nucl. Acids Res., 2003 Jan 1;31(1):207-11.
20. Kolesov, G., Mewes, H.-W., Frishman, D. (2002). SNAPper: gene order predicts gene function. Bioinformatics, 2002 Jul;18(7):1017-9
21. Kolesov, G, Mewes, H.-W, Frishman, D. Prediction of gene function in bacterial genomes based on context information. Ernst Schering Research Foundation Workshop Volume 38: Bioinformatics and Genome Analysis. Editors: H.-W. Mewes, B. Weiss, H. Seidel, Book Chapter, Springer-Verlag, Berlin Heidelberg, Chapter 3, 2002.
22. Schoof H, Zaccaria P, Gundlach H, Lemcke K, Rudd S, Kolesov G, Arnold R, Mewes HW, Mayer KF. (2002). MIPS Arabidopsis thaliana Database (MATDB): an integrated biological knowledge resource based on the first complete plant genome. Nucleic Acids Res. 2002 Jan 1;30(1):91-3.
23. **Kolesov G, Mewes H.-W, Frishman D. (2001). SNAPping up functionally related genes based on context information: a colinearity-free approach. J Mol Biol., 2001 Aug 24;311(4):639-56.**
24. **..., Kolesov G, ..., Sequence and analysis of chromosome 5 of the plant Arabidopsis thaliana. Nature, 2000, 408, 823-6.**
25. Anan'ko EA, Kolpakov FA, Kolesov GB, Kolchanov NA. [Automatic generation of gene network schemes based on their formalized description in the GeneNet database] Biofizika. 1999 Jul-Aug;44(4):628-31. Russian.
26. Kolpakov FA, Ananko EA, Kolesov GB, Kolchanov NA. (1998). GeneNet: a gene network database and its automated visualization. Bioinformatics, 14, 529-37.
27. ..., Kolesov, G.B. and co-workers, (1998). GeneExpress: a computer system for description, analysis, and recognition of regulatory sequences in eukaryotic genome. Proc Int Conf Intell Syst Mol Biol. 6, 95-104.

