ANATOLI A. KORKIN

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SUMMARY

Associate research professor at Arizona State University and president of Nano & Giga Solutions. Computational chemist, materials scientist and project manager with extensive experience in academic and industrial research. Conducted studies in process and material design for advanced microelectronics, high energy density materials, physical chemistry of main group and transition elements, biologically active materials and photo biosensors. Published 100+ papers in peer reviewed journals. Last five years focused on research and consulting in the area of nanotechnology and computational materials design. Current research focus - materials and devices for solar energy applications. Strengths include technical skills, project management and world wide professional networking.

KEY QUALIFICATIONS

Technical: Expertise in the broad areas of computational and physical chemistry with applications in microelectronics, high energy materials (rocket propellants, explosives and metastable compounds), gas and solid state chemistry, main group and transition elements chemistry, biologically active molecules and biosensors.

Business: Remote and complex project management, business development (team building, strategy development, technical due diligence), event organizing.

Software: Knowledge of numerous computational chemistry and materials science programs, such as GAUSSIAN, Cerius2/Molecular Studio, GAMESS, SIESTA, VASP. Co-developer of Khimera and SageMD programs.

Computers: User knowledge of UNIX, MS Windows, Linux and Internet tools.

Writing: Co-author of more than 100 scientific papers published in peer-reviewed journals, and co-editor of three books and five special journal issues.

Languages: Fluent in Russian, English, German, good knowledge of French.

Others: Editorial, program and team management, remote (internet based) professional networking, fund raising.

PROFESSIONAL APPOINTMENTS

2007-Present: Associate research professor, Department of Chemistry and Biochemistry, Arizona State Univercity, Tempe Arizona.

- ***Current projects***

- Development of Russian Science Technology and Education Center (RUSTEC)
- Computational design of thin film materials and devices for photovoltaic applications
- Educational web portal ASDN.NET

2003-Present President, Nano & Giga Solutions, Gilbert, Arizona (http://nanoandgiga.com/)
Nano and Giga Solutions is an independent start-up company, which provides products and services in the area of computational chemistry, material science and nanotechnology. The Company offers consulting, research and software development in the area of computational chemistry, materials science and nanotechnology.

- ***Current projects:***

- Development of the educational web portal in atomic scale materials design (ASDN.NET)
- Organizing conference series "Nano & Giga Forum"
- Consulting in international projects in education, science and innovations.

- ***Past projects:***

- Nano and Giga Challenges in Electronics and Photonics (NGC2009) – international conference;
- Atomic scale modeling of Si-SiO_2 interface for future electronic devices in collaboration with SEMATECH International (Dr. G. Bersuker), University of Florida (Prof. R.J. Bartlett), Tyndall National Institute, Ireland (Dr. J. Greer);
- Atomic scale modeling of high-k dielectric materials and interfaces in collaboration with SEMATECH International (Dr. H. Huff, Dr. G. Bersuker) and University of Tokyo (Prof. Koichi Yamashita);
- Team and strategy building for a start-up company in Bay Area.

- ***Expertise offered (individual and with network partners):***
  - Business development and consulting – project management, team building, strategy development, and technical due diligence
  - Research and consulting in different areas of computational chemistry and materials design.
  - Atomic scale process, materials and device design for advanced electronics (silicon oxide, high-k, and low-k oxides) and their interfaces with semiconductors and metals.
  - Atomic scale design of future electronic devices (molecule/solid state interfaces, quantum dots and wires).
  - Modeling and simulation of the hydrogen storage and fuel cells
  - Software development for quantum transport in nanoCMOS and nano and molecular devices.

1997-2003 Project Manager and Senior Research Scientist (staff engineer), DigitalDNA Labs, Motorola, Inc., Tempe, Arizona.

Conducted research and project management in modeling and simulation of the mechanism and kinetics of chemical vapor deposition (ALD and CVD), the structure, stability and electronic properties of advanced electronic materials, thin films, interfaces and electronic devices supervised two groups of contractors in Russia. Published 28 papers in international peer-reviewed journals. Jointly with Motorola and external contractor teams:

- Developed the mechanism and kinetics of ALD and CVD of Si_3N_4, SiO_xN_y (silicon oxinitride), TiN, ZrO_2, HfO_2 and Al_2O_3, which have been used by DigitalDNA Lab engineers to design and optimize process and chemical reactors;
- Developed two commercial software packages, Khimera (mechanism and chemical kinetics) and Sage MD (atomic scale material design and molecular dynamics), for general use in material and process design;
- Developed novel process design for vapor jet Al_2O_3 deposition to obtain H-, C-, Cl-free aluminum oxide films for gate oxide and passive device applications.

1995-1997 Research Associate in the group of Prof. Rodney J. Bartlett, Quantum Theory Project, University of Florida, Gainesville, Florida,

Conducted quantum chemical studies of processes and materials, such as high energy density materials (HEDM) and metastable molecules.

- Established decomposition pathways for the series of experimentally known and hypothetical explosives and propellants;
- Discovered theoretically and studied computationally new high energy density materials: $C_3N_6O_6$ (trinitrotiazine), CN_2O (nitroso cyanide, CN_2O_2 (nitro cyanide), NO_4^+ (tetraoxynitryl cation), and O_4 (oxygen dimer).

1993-1995 Research Fellow in the group of Prof. Kurt Schaffner; Max-Planck Institut für Strahlenchemie, Mülheim /Ruhr, Germany.

Applied molecular modeling and simulation to study biologically active oligopyrroles. Conducted vibrational analyses of the phytochrome's chromophore and model species.

- Established the nature of active IR and Raman vibrational modes to assist the functional studies of the phytochromes;
- Developed a computational model of conformational response of the chromophore on photo excitation.

1991-1993 Alexander-von-Humboldt Fellow in the group of Prof. P.v.R. Schleyer; Friedrich-Alexander University of Erlangen-Nurnberg, Erlangen, Germany.

Sudied π bond energies in conjugated and aromatic carbon and silicon molecules and structure-property correlations in a series of molecules containing boron, carbon and silicon.

- Developed a model of radical stabilization effect on energy and reactivity of π bonds;
- Established effect of hypercongugation on structure and reactivity of aromatic silicon compounds;
- Established structure and reactivity of series of small boron hydrides.

1981-1991 Senior Researcher, Institute of Physiologically Active Substances, Russian Academy of Sciences, Chernogolovka, Moscow Region , Russia.

Studied orbital models of hypervalent and low coordinated phosphorus, silicon and sulfur compounds and biological activity of phosphororganic compounds.

- Developed a theoretical model of structure - reactivity relations in phospholanes and phosporanes;
- Developed a mechanism of acid-catalized cleavage of PN bonds;
- Developed a stereoelectronic model for structure - properties relations in silicon and phosphorus compounds;
- Computed structures and heats of formations of metastable intermediates in pyrolysis of biologically active phosphorus compounds.

HIGHER EDUCATION

Ph.D. in Physics

Graduate studies at the Moscow Lomonosov State University; *Thesis topic:* Structure of Photosynthetic Molecules and the Mechanism of the Primary Charge Separation in the Reaction Centers of Photosynthetic Bacteria, 1981

M.S. in chemistry

Undergraduate studies in Moscow Mendeleev Technical University; *Thesis topic:* Quantum Chemical Models of the Electron Density in the Crystals of HCOOLi-H_2O, 1978

PROFESSIONAL REFERENCES

Prof. William Petruskey: Arizona State University, Tempe, Arizona, USA, Phone: +1-480-965-4430; Fax: +1 (480) 965-2747; E.mail: wpetuskey@asu.edu.

Dr. Stephen Goodnick: Arizona State University, Tempe, Arizona, USA; Phone: 1 (480) 965-1125; Fax: 1(480) 965-8293; E.mail: Stephen.goodnick@asu.edu

Dr. Bruce Garrett: Pacific Northwest National Laboratory, 902 Battelle Blvd, Richland WA 99352; Phone: 1 (509) 372-6344; Fax: (509) 375-6776; E-mail: bruce.garrett@pnl.gov

Prof. Rodney J. Bartlett: Quantum Theory Project, University of Florida, Gainesville, FL, 32611; Phone: 1 (352) 392-1597; Fax: +1 (352) 392-8722; E.mail: bartlett@qtp.ufl.edu

Dr. Gennadi Bersuker: SEMATECH International, 2706 Montopolis Dr, Austin, TX 78741; Phone: 1 (512) 356 3334; Fax: 1 (512) 356 7045; E.mail: Gennadi.Bersuker@sematech.org

Dr. Alex Demkov: Freescale Semiconductor, Inc. K10, 3501 Ed Bluestein Blvd, Austin TX 78721, USA; Phone: 1 (512) 933-6863; Fax: +1 (512) 933-8770; e.mail: alex.demkov@freescale.com

Prof. Gernot Frenking: Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Strasse, Marburg, FRG D-35032; Phone: +(49) 6421-285563; Fax: +(49) 6421-282189; E.mail: frenking@chemie.uni-marburg.de

Dr. David Gilmer: Freescale Semiconductor, Inc., K10, 3501 Ed Bluestein Blvd, Austin, TX, 78721; Phone: 1 (512) 933-8762; Fax: 1 (512) 933-6962; E.mail: david.gilmer@freescale.com

Dr. Jan Labanowski: Computational Chemistry List, LTD, 2715 Westmont Blvd, Columbus, Ohio, 43221, USA ; Phone: 1 (614) 487-8373; FAX 1 (614) 487-9838; E.mai: jkl@ccl.net

Prof. Paul von Rague Schleyer: Computational Chemistry Annex, The University of Georgia, Athens, GA 30602-2525 USA; Phone: (+1) 706 542 7510; Fax: (+1) 706 542 7514; e-mail: schleyer@chem.uga.edu

Addendum

AWARDS

Humboldt Fellowship from the Foreign Ministry of Germany
Research Award from the National Sciences and Engineering Research Council of Canada
Eighteen Silver Quill Awards and Golden Quill Award from Motorola

PROFESSSIONAL ACTIVITIES

2011 General chair of the symposium and summer school on Nano and Giga Challenges in Electronics, Photonics and Renewable Energy (NGC2011), Moscow-zelenograd, Russia, September 10-14, 2011 (http://asdn.net/ngc2011)

2010 Invited speaker at the XIIIth Tomsk Innovation Forum, Tomsk, Russia, May 20,21, 2010

2010 Invited speaker and Program Committee member of international Nano Technology Education Conference, Moscow, Russia, May 18-20, 2010

2009 Invited speaker at the international school for young scientists in innovations Management, Nozhnij Novgorod, Russia, October 26-30, 2009. http://www.crdf-techin.ru/ru/projects/mezhdunarodnaia_nauchnaia_shkola_po_innovatsionnomu_menedzhmentu/

2009 Co-chairman of the of the symposium and summer school on Nano and Giga Challenges in Electronics, Photonics and Renewable Energy (NGC2009) and 14th Canadian Semiconductor Technology Conference (CSTC2009), Hamilton, Ontario, Canada, August 10-14 (http://asdn.net/ngc2009/)

2007 Visiting Senior Scientist, Chemical System Engineering, University of Tokyo.

2007 Invited speaker at Micro-NanoSystems European Nework meeting, Bucharest Romania, May 23-25 (http://www.minos-euro.net/23-25may2007/programme.htm)

2007 Co-chairman of the program committee of the symposium and summer school on Nano and Giga Challenges in Electronics and Photonics, Phoenix, Arizona, March 12-16 (http://asdn.net/ngc2007/)

2006 Invited talk, 209th ECS Meeting, Denver, Colorado, May 7-12, 2006.

http://ecsmeet1.peerx-press.org/jsp/mas/reportTechProg.jsp?MEETING_ID=601&SYM_ID=116

2006 Invited lecture, Materials Science & Technology Institute (EMPA), Zurich, Switzerland, January 30.

2006 Invited lecture, University of Luis Pasteur, Srasbourg, France, January 27.

2006 Visiting Scientist, University of Paderborn, Germany, January 15 – February 15.

2005 Co-chairman of the symposium "Combinatorial Methods and Informatics in Materials Science" at the MRS 2005 fall meeting, Boston, MA http://www.mrs.org/meetings/fall2005/program/f05_cfp_ll.html

2005 Invited lecture in University of California, Berkeley, California, October 6.

2005 Invited lecture in Stanford Research Institute (SRI International), Menlo Park, California, October 4.

2005 Invited speaker, Nano Electronics & Photonics Forum, July 14, Palo Alto, CA. **h**ttp://www.nanotech-now.com/news.cgi?story_id=09698

2005 Visiting Senior Scientist, Chemical System Engineering, University of Tokyo.

2005 Invited lecture in Florida International University. Hosted by the IEEE chapter. http://www.eng.fiu.edu/HTML2003/news/Korkin%20Feb%2025%202005.pdf

2004 Visiting senior researcher at the Quantum Theory Project, University of Florida, Gainesville, Florida

2004 Visiting senior researcher at the National Microelectronic Research Center, Cork, Ireland.

2004 Chairman of the Program Committee of the Symposium and Summer School on Nano and Giga Challenges in Microelectronics (MGCM2004), September 13-17, Krakow, Poland: http://asdn.net/ngcm2004/

2004 Co-chairman of the Atomic Scale Materials Design: Modeling and Characterization symposium at the 2004 E-MRS Spring Meeting, May 24-28, Strasbourg, France: http://www-emrs.c-strasbourg.fr/2004_SPRING/2004_h.pdf

2003 Co-chairman of the Atomic Scale Material Design Modeling & Simulation symposium at the annual Meeting of the Material Research Society, MRS 2003 Fall Meeting, December 1-5, Boston, MA: http://www.mrs.org/meetings/fall2003/symp_kk.html

2003 Co-chairman of the US-Russian Workshop on Software Design: Bridging Atomic and Macroscopic Scales in Materials, Process and Device Design, November 13-15, Tempe, AZ: http://www.atomicscaledesign.net/swn2003/

2002 Co-chairman of the Atomic Scale Materials Design Symposium at E-MRS Spring Meeting, June 17-21, Strasbourg, France: http://www-emrs.c-strasbourg.fr/2002_Book_Abs/02_Prog_Av2.pdf

2002 Co-chairman of the Symposium and Summer School on Nano and Giga Challenges in Microelectronics Research and Opportunities in Russia, September 10-13, 2002, Moscow, Russia: http://www.asdn.net/moscow/

2002 Co-chairman of the Symposium on Software Development for Process and Materials Design, September 15-16, Moscow Russia: http://www.asdn.net/moscow/software.shtml

2001-2003 Project leader of the Motorola team in the international project in modeling high-k materials (HIKE). The project has been funded by European parliament and includes groups from Infineon (Germany), National Microelectronic Research Center (Ireland), University Colleague London (UK) and LAAS CNRS (France): http://www.nmrc.ie/hike/

2001 Leader of the Motorola team in a international project for joint experimental and theoretical studies of ZrO_2 ALD and film structure and properties. The project includes the research company Kintech in Moscow and experimental groups at the Universities of Helsiniki, Finland and Tartu, Estonia

2001-2003 Supervisor of the Molecular Dynamics group at the Sarov Open Computing Center (DOE funded project): http://www.sarovlabs.com/

2000-2003 Supervisor of the Surface Chemistry group at the Kurchatov Institute, Moscow, a subcontractor of Motorola: http://www.kintech.ru (project funded by Motorola and DOE)

2000 Co-chairman of the Motorola-VNIIEF (Russian Nuclear Research Center) workshop, June 14-16, Sarov, Russia: http://www.sarovlabs.com

2000 Member of the Advisory Committee for the Alliance for Nonlinear Optics

1999 Visiting professor in the Theoretical Chemistry Center of the University of Marburg; host Prof. G. Frenking: http://www.chemie.uni-marburg.de/~frenking/group/guests.html

1998-2000 Co-supervisor of the PhD research of Magdalena Siodmiak (jointly with Prof. G. Frenking) at the University of Marburg, Germany. PhD Thesis: Theoretical Study

of Chemical Vapor Deposition of Transition Metal Compounds“ http://archiv.ub.uni-marburg.de/diss/z2001/0084/volltext.html

1997-2001 Supervisor of the Chemical Kinetics research group at Soft-Tec, LTD, a subcontractor of Motorola: http://www.soft-tec.ru/

1995 Chief Scientist, ACES Q.C., University of Florida, Gainesville, FL, 32611: http://www.acesqc.com/

1994 Visiting Professor, Dalhousie University, Halifax, Canada; host Prof. R. Boyd: http://www.chem.dal.ca/faculty/rjb/ppd.html

1991 Scientific Director, GERUS company; Institute of Elemento-Organic Compounds Russian Acad.Sci., Vavilov St., 28, Moscow 117813, Russia

1989-1991 Scientific Secretary of the Soviet Union Branch of World Association of Theoretically Oriented Chemists (WATOC): http://www.ch.ic.ac.uk/watoc/

1989-1991 Scientific Secretary of the Theoretical Chemistry Section of the Mendeleev Chemical society of Soviet Union.

1988 Chairman, Regional Soviet Union Conference on Stereoelectronic Effects in the Chemistry of IV-VI Group Elements (Anapa, September, 1989)

LIST OF PUBLICATIONS

Editorial: Books & Journal Issues:

1. Computational Materials Science, 2003, v.28, No.2, Eds. J. Greer, A. Korkin, J. Labanowski.

2. Microelectronic Engineering, 2003, v. 69, No 2-4, Eds. B. Aronzon, A. Demkov, K. Golant, J. Greer, E. Gusev, A. Korkin, J. Labanowski, D. Resnick.

3. Nano and Giga Challenges in Microelectronics, Eds, J. Greer, A. Korkin, J. Labanowski. Elsevier, Amsterdam , 2003. http://www.elsevier.com/locate/isbn/0444514945

4. Computational Materials Science, 2005, v. 33, No 1-3, Eds. A. Esteve, M. Djafari-Rouhani, J. Greer, A. Korkin.

5. Microelectronic Engineering, 2005, v. 81, No 2-4, Eds. A. Korkin, A. Burian, J. Labanowski, S. Luryi, N. Perov, M. Shur, M. Szymonski.

6. International Journal of Nanotechnology, v. 2, No. 3-4, 2005. Eds. A. Korkin, J. Labanowski, A. Volinsky,

7. Combinatorial Methods and Informatics in Materials Science, MRS Symposium Proceedings, vol. 894, 2006. Eds. M.J. Fasolka, Qi Wang, R. A. Potyrailo, T. Chikyow, U.S. Schubert, A. Korkin.

8. Nanotechnology for Electronic Materials and Devices, Eds, A. Korkin, E. Gusev, J. Labanowski, S. Luryi, Springer, N-Y, 2007.

9. Solid State Electronics, Eds, S. Goodnick, A. Korkin, T. Naito, N. Peyghambarian , v. 51, N0.10, 2007

10. Nanotechnology, Eds, P. Krstic, E. Forzani, NJ Tao, A. Korkin, v.18, No. 42, 2007

11. Nanoelectronics and Photonics, Eds. A. Korkin, F. Rosei, Springer 2008.

12. Nanotechnology, Eds, S. Goodnick, A. Korkin , P. Krstic, P. Mascher, J.Preston, and A. Zaslavsky, v. 21, No. 13, 2010

13. Nano Scale Reseach Letters, Eds. A. Korkin, P. Krstic, Z. Miskovic, H. Yu and I. Zhitomirsky, v. 5, No. 3, 2010.

14. Nanotechnology for electronics, photonics, and renewable energy, Eds, A. Korkin, P. Krstic, and J. Wells, Springer, 2010.

15. Nano Scale Research Letters. Eds. David Gilmer, A. Korkin, P. Krstic,Yu. Lozovik, and D. Narducci. *In ptress.*

16. Nanotechnology for for electronics, photonics, and renewable energy, Eds, A. Korkin and D. Lockwood, Springer, *in press*.

Contributions in Books & Proceedings:

1.. Korkin, A.A. Theoretical Models for "Unusual" Coordination at Silicon. In Chem. Technol. Silicon Tin, Proc. Asian Network Anal. Inorg. Chem. Int. Conf. Silicon Tin, 1st, Eds, Kumar Das, V.G.; Ng, Seik Weng; Gielen, M., Oxford Univ. Press: Oxford, UK, 1992, 459-469.

2. Bartlett, R.J.; Nooijen, M.; Gwaltney, S.; Korkin, A.A. New Methods for Excited States. In Proceedings of the High Energy Density Matter (HEDM) Contractors' Conference Held in 1-3 June 1997 in Chantilly, VA. Adwards Air Force Base, 1998, pp. 37-42.

3. Tanpipat, N.; Andzelm, J.; Delley, B.; Korkin, A.A.; Demkov, A. Atomistic Modeling of Chemical Vapor Deposition: NO on the Si(001) (2x1) Reconstructed Surface. Proceedings of the Fifteenth International Symposium on Chemical Vapor Deposition. The Electrochemical Society, Inc., Pennington, NJ, 2000-13: http://www.aiche.org/conferences/techprogram/paperdetail.asp?PaperID=251&DSN=annual99

4. Siodmiak, M.; Frenking, G.; Korkin, A. Theoretical ab initio Study of TiCl4 Ammonolysis: Gas Phase Reactions of TiN Chemical Vapor Deposition. In Highlights in Computational Chemistry, Springer Verlag, 2001, p. 413. http://www.booksmatter.com/b354067876X.htm

5. Gutowski, M.; Jaffe, J.E.; Chun-Li Liu; Stoker, M.; Korkin, A.; Veteran, J.L.; O'Meara, D.L.; Misra, V.; Ho, P.S. Oxides, silicides, and silicates of zirconium and hafnium; density functional theory study Mater. Res. Soc. Proceedings, 2002, 716, 267-272.

6. Bagatur'yants A.; Korkin, A.; Novoselov, K.; Savchenko, L.; Umanski, S. Integrated Approach to Atomistic Simulation of Film Deposition Processes. In COMPUTATIONAL MATERIALS SCIENCE, Eds, C.R.A Catlow, E. Kototmin, IOS Press, Amsterdam, 2003, pp. 388-418.

7. Bagatur'yants, A.A.; Minushev, A.Kh.; Novoselov, K.P.; Safonov, A.A.; Umanski, S. Ya.; Vladimirov, A.S.; Korkin, A.A. Atomistic Simulation of Si_3N_4 CVD from Dichlorosilane and NH_3. In Predictive Simulation of Semiconductor Processing: Status and Challenges, Eds, J. Dabrowski, E. R. Weber, Springer Series in Materials Science, Vol. 72, Springer Verlag, 2004, pp 295-356.

8. Bazhanov, D. I.; Safonov, A. A.; Bagatur'yants, A. A.; Korkin, A. A. The structure and electronic properties of Zr and Hf nitrides and oxynitrides. In Micro- and Nanoelectronics 2003. Eds K. Valiev, A. Orlikovsky, Proceedings of the SPIE, Volume 5401, pp. 418-425 (2004). http://adsabs.harvard.edu/abs/2004SPIE.5401..418B

9. Bersuker, G.; Peterson, J.; Barnett, J.; Korkin, A.; Sim, J.H.; Choi, R.; Lee, B.H.; Greer, J.; Lysaght, P.; Huff, H.R. Properties of the Intermediate Layer in the High-k Gate Stack and Transistor Performance. Proc. 2005 ECS Spring Meeting, 2005-05, 141-145.

10. Knizhnik, A.A.; Iskandarova, I.M.; Bagatur'yants, A.A.; Potapkin, B.V.; Fonseca, L.R.C.; Korkin, A.A. Metal Screaning for CMOS Application through *AB-INITIO* Interface Work Function Calculations. Proceedings of 20th Symposium on Microelectronics and Devices (SBMICRO 2005), September 4-7, 2005, Florianopolis, Brazil, 165-179.

11. Bartlett, R.J.; D.E. Taylor, D.E.; Korkin, A. Achieving Predictive Simulations with Quantum Mechanical Forces via Transfer Hamiltonian: Problems and Prospects, in Handbook of Materials Modeling, Vol. 1: Methods and Models, Ed. S. Yip, Springer, Berlin, Chapter 1.3, 2005.

13. Henderson, T.M.; Greer, J.C.; Bersuker, G.; Korkin. A.; Bartlett, R.J. Effect of Chemical Environment and Strain on Oxygen Formation Energy at Silicon – Silicon Oxide Interfaces. In Defects in Advanced High-k Dielectric Nano-Electronic Semiconductor Devices, Ed. E. Gusev, Springer, 2006, pp 373-384.

14. Korkin A.; Kamisaka, H.; Yamashita, K.; Safonov, A.; Bagaturyants, A Computational DFT Study of $ZrSiO_4$ Polymorphs: Potential Microelectronic, Nuclear Safety and Geological Implications. Materials Research Society Symposium Proceedings, Vol. 84, 283-294 (2006).

15. Greer, J.C; Hendersen, T.M.; Bersuker, G.; Bartlett R.J.; Korkin A.A. Oxygen Vacancies at $Si(100)/SiO_2$ Interfaces. Electrochemical Society Transactions, 2, pp. 205-211 (2006).

16. Bersuker, G.; Hun Lee B.; Huff H.R,; Korkin, A. Novel Materials for Future Transistor Generations. In Nanotechnology for Electronic Materials and Devices (Nanostructure Science and Technology series), Eds, E. Gusev, A. Korkin, J. Labanowski, S. Luryi, Springer, N-Y, pp. 199-222 (2006).

Papers in Peer Reviewed Journals:

1.Ozerov, R.P.; Tsirelson, V.G.; Ionov S.P.; Korkin A.A.; Zavodnik B.E.; Fomicheva, E.B. Studies of the Valent Electrons Distribution in Crystals .III. Experimental and Theoretical Investigation of the Electronic Density in HCOOLi-D_2O. Kristallographiya, 1981, 28, 42-46 [Russian].

2. Korkin, A.A.; Ionov, S.P. Physicochemical Principles of the Structure and Functioning of the Reaction Centers of Photosynthesising Bacteria. I. Photochemical Processes and Electronic Structure of the Pigments. Russian J. Phys. Chem., 1981, 55 (12), 1707-1714.

3. Korkin, A.A.; Ionov, S.P. Physicochemical Principles of the Structure and Functioning of the Reaction Centers of Photosynthesising Bacteria. II. Organization of the Reaction of Pigments in the Reaction Centers. Russ. J. Phys. Chem., 1982, 56, 317-323.

4. Korkin, A.A.; Ionov S.P. Physicochemical Principles of the Structure and Functioning of the Reaction Centers of Photosynthesizing Bacteria. III. Models of Electron-Transfer Agents and Primary Processes. Russ. J. Phys. Chem., 1982, 56 (6), 1343-1354.

5. Tsvetkov, E.N.; Korkin, A.A. Antibonding Orbitals and Their Role in Electronic Interactions in Compounds with a Phosphoryl Group. Russ. J. Theor. Exp. Chem., 1985, 21, 36-42.

6. Tsvetkov, E.N.; Korkin A.A. Certain Characteristic Features of Phospholane and Phosphorinane systems and Electrophilicity of Antibonding Orbitals of Phosphorus Atom. Russ. J. Theor. Exp. Chem., 1985, 21, 152-157.

7. Tsvetkov, E.N.; Korkin A.A. Dimerization of Iminophosphoryl Compounds and Electrophilicity of Antibonding Orbitals of the Phosphorus Atom. Russ. J. Theor. Exp. Chem., 1985, 21, 512-519.

8. Korkin A.A.; Tsvetkov E.N. Mechanism of Acid-Catalyzed of Cleavage of P-N Bond. Russ. J. Gen. Chem. USSR, 1987, 57(II), 1929-1932.

9. Chernega A.N.; Korkin A.A.; Antipin, M.Yu.; Struchkov Yu.T. X-Ray Diffraction and Quantum Chemical Data on the Phosphorus-Nitrogen Double Bonds of Dicoordinated and Tetracoordinated Phosphorus. J. Gen. Chem. USSR, 1988, 58(II), 1823-1832.

10. Korkin, A.A.; Tsvetkov, E.N. Theoretical Investigation of the Interaction between the H_nX-YH_m molecules and Electron Acceptors. The ab initio Study of the Effect of Protonation on the P-N Bond in PH_2NH_2. Bull. Soc. Chim. France, 1988, 335-338.

11. Korkin, A.A., Aksinenko, N.A., Tsvetkov, E.N. Quantum Chemical Simulation of the Hypervalent Bonding in Phosphatranes. Phosphorus and Sulfur, 1988, 40, 149-154.

12. Korkin, A.A.; Tsvetkov, E.N. Quantum Chemical Study of the Donor-Acceptor Interactions between Silicon, Phosphorus and Sulfur Halides with the Carbonyl Group of Formaldehyde. Bull. Acad. Sci. USSR. Div. Chem. Sci., 1988, 37, 500-502.

13. Korkin, A.A.; Aksinenko N.A.; Tsvetkov, E.N. Quantum Chemical Study of the Donor-Acceptor Interactions between Silicon, Phosphorus and Sulfur Halides and Ammonia, Bull. Acad. Sci. USSR. Div. Chem. Sci., 1988, 37, 503-505.

14. Korkin, A.A.; Aksinenko, N.A.; Tsvetkov, E.N. Semi empirical Models of the Trans-annular Bond in Silatranes and Phosphatranes. Bull. Acad. Sci. USSR. Div. Chem. Sci., 1988, 37, 1846-1851.

15. Korkin, A.A.; Mebel, A.M.; Borisov, E.V. Nonempirical Study of Oxyphosphonitride (PNO) Isomers. Bull. Acad. Sci. USSR. Div. Chem. Sci., 1988, 37, 780-783.

16. Chernega, A.N.; Korkin, A.A.; Antipin, M.Yu.; Struchkov, Yu.T.; Ruban, A.V.; Romanenko, V.D. Steric and Electronic Structure of Phosphinimines According to the Results of X-Ray Investigations and Nonempirical Quantum-Chemical Calculations. Russ. J. Gen. Chem. 1989, 59, 2010-2017.

17. Korkin, A.A.; Tsvetkov, E.N. A Quantum-Chemical Study of the Influence of Protonation on Intramolecular Interactions in the Molecules of Hydrazine, Aminophosphine, and Diphosphine. Russ. J. Inorg. Chem. 1989, 34, 161-164.

18. Korkin, A.A.; Tsvetkov, E.N. Dimerization of Iminiphosphoranes. Russ. J. Gen. Chem. 1989, 59, 849-851.

19. Chernega, A.N.; Korkin, A.A.; Antipin, M.Yu.; Struchkov, Yu.T.; Molecular and Electronic Structure of Iminophosphines. Phosphorus and Sulfur, 1990, 49/50, 345-348.

20. Korkin A.A. Double Bonds in the Second and Third Periods. Ab initio Study of the Conjugation in $H_nX{=}YH_m$-ZH (X,Y=C, N, Si, and P; Z=B, and N; n=1,2; m=0,1). Int. J. Quantum Chem., 1990, 38, 245-252.

21. Korkin, A.A.; Tsvetkov, E.N. Nonempirical Study of the Addition of F^+ to H_2PNH_2 Russ. J. Gen. Chem. 1990, 60, 2392-2395.

22. Korkin A.A. Stereoelectronic Effects in Main Groups IV-VI Compounds. Metalloorganicheskaya Khimia, 1990, 3, 969-975 [Russian].

23. Korkin, A.A.; Mebel, A.M. Comparative Ab Initio Study of the Conjugation in Iminophosphines and Iminophosphoranes. Metalloorganicheskaya Khimia, 1990, 3, 1005-1011 [Russian].

24. Brel', V.K.; Gakh, A.A.; Zhdankin, V.V.; Zefirov, N.S.; Koz'min, A.S.; Korkin, A.A.; Kuatelidze, T.G.; Caple, P.; Lermontov, S.A.; Plokhikh, I.G.; Safronov, S.O.; Stang, P.J.; Chovnikova, N.G. 10-Electron Reagents - Derivatives of Iodin (III), Xenon (II), Selenium (IV), Tellurium (IV) in Organic Synthesis. Dokl. Akademii Nauk USSR, 1990, 313, 1131-1135 [Russian].

25. Korkin, A.A.; Chernega, A.N.; Aksinenko, N.E.; Ruban, A.V.; Romanenko, V.D. Molecular and Electronic Structure of P-Halo-Lamda3-Imonoohosphines. Russ. J. Gen. Chem. 1990, 60, 2201-2207.

26. Budyka, M.F.; Laukhina, O.D.; Korkin, A.A.; Alfimov, M.V. Study of the Thermal Stages of Photoiniciated Cyclization of Diarilamines with Polyhalogenated methanes. Bull. Acad. Sci. USSR. Div. Chem. Sci., 1991, 564-569.

27. Chernega, A.N.; Korkin A.A.; Antipin, M.Yu.; Struchkov, Yu.T.; Ruban, A.V.; Romanenko, V.D.; Markovski, L.N. Peculiarities of P_{π}-P_{π} Conjugation in Aminosubstituted Phosphaalkenes. Heteroatom Chem., 1991, 2, 229-241.

28. Korkin, A.A. Stereoelectronic Effects in Silicon, Phosphorus, and Sulfur Molecules. Quantum-Chemical Calculations and Qualitative Orbital Models. Russian Chemical Reviews, 1992, 61 (5), 473-483; http://www.turpion.org/php/paper.phtml?journal_id=rc&paper_id=957

29. Borisov, E.A.; Mebel, A.M.; Knyazev, V.B.; Zabrodin, V.B. Korkin, A.A. Comparative Nonempirical Study and Isodesmic Calculations of Heats of Formation of HNCO and HPCO isomers. Bull. Acad. Sci. USSR Div. Chem. Sci. 1992, 1222-1226.

30. Korkin, A.A.; Glukhovtsev, M.N.; Schleyer, P.v.R. Polysilaanalogs of Aromatic Hydrocarbon Ions: Structures and Energies of $Si_3H_3^+$, $Si_4H_4^{2+}$, and $Si_5H_5^-$. Int. J. Quant. Chem., 1992, 46, 137-144.

31. Korkin, A.A.; Schleyer, P.v.R. Trisilaallyl Anion Structures. Is Conjugation effective? J. Amer. Chem. Soc., 1992 , 114, 8720-8722.

32. Dransfeld, A.; Korkin, A.A.; Salzner, U; Schleyer, P.v.R. Application of Ab Initio ^{31}P NMR Chemical Shifts Calculations. Phospphorus Sulfur, 1993, 77, 260.

33. Chernega, A.N.; Koidan, G.N.; Marchenko, A.P.; Korkin, A.A. The Structural Evidence for P_{π}-P_{π} Conjugation in Aminosubstituted Phosphaalkynes. Heteroatom Chem., 1993, 4, No.3, 1-4.

34. Chernega, A.N.; Korkin, A.A. Substution effects on Multiple Phosphorus-Carbon Bond. Phosphorus, Sulfur, and Silicon, 1993, 76, 65.

35. Korkin, A.A.; Schleyer, P.v.R.; Boyd, R.J. Theoretical Study of N_2CO Isomers: New Candidates for High Energy Materials. Chem. Phys. Letters, 1994, 227, 312-320.

36. Korkin, A.A.; Schleyer, P.v.R.; McKee, M.L. Theoretical Ab Initio Study of Neutral and Charged B_3H_n Species. The Importance of Aromaticity in Determining the Structural Preferences. Inorg. Chem. 1995, 34, 961-977.

37. Matysik, J.; Hildebrandt, P.; Smit, K.; Korkin, A.; Mark, F.; Gärtner, W.; Braslavsky, S.E.; Schaffner, K.; Schrader, B. Vibrational Analysis of Biliverdin Dimethyl Ester. J. Mol. Structure, 1995, 348, 225-228.

38. Korkin, A.; Schleyer, P.v.R.; Arx, U.v.; Lauber, R.; Keese, R. The Aromatic Diboracyclopropenyl (dyboriranyl) anion. Struct. Chem. 1995, 6, 225-228.

39. Jemmis, E.D.; Srinivas, G.N.; Leszczynski, J.; Kapp, J.; Korkin, A.A.; Schleyer, P.v.R. Group 14 Analogs of the Cyclopropenuim Ion: Do They Favor Classical Aromatic Structures? J. Am. Chem. Soc. 1995, 117, 11361-11362.

40. Korkin, A.A.; Murashov, V.; Leszczynski, J.; Schleyer, P.v.R. Theoretical Study of Cyclic $Si_5H_5^+$ Structural Isomers. Is There Any Analogy with the Corresponding Carbon Species? J. Phys. Chem. 1995, 99, 17742-17747.

41. Chernega, A.N.; Korkin, A. A. ; Romanenko, V.D. Particularities of Geometries and Electronic Structure of λ^3-Phosphines. Z. Obstchei Khimii 1995, 65, 1823-1833 [Russian].

42. Korkin, A.A.; Balkova, A.; Bartlett, R.J.; Boyd, R.J.; Schleyer, P.v.R. The Twenty Eight-Electron Tetraatomic Molecules. A Challenge for Computational and Experimental Chemistry. J. Phys. Chem. 1996, 100, 5702-5714.

43. Korkin, A.; Mark, F.; Schaffner, K.; Gorb, L.; Leszczynski, J. Theoretical Ab Initio and Semi-Empirical Studies of Biologically Important Di- and Oligopyrrolic Compounds. Pyrromethene and Protonated Pyrromethene. J. Mol.Struct. THEOCHEM 1996, 388, 121-137.

44. Korkin, A.A.; Murashov, V.V.; Leszczynski, J.; Schleyer, P.v.R. Trisilallyl Cation and Related Structures. Departures from the Corresponding Carbon Species. J. Mol. Struct. THEOCHEM 1996, 388, 43-49.

45. Korkin, A.A.; Leszczynski, J.; Bartlett, R.J. Theoretical Ab Initio Study of CN_2O_2 Structures: Prediction of Nitryl Cyanide as a High-Energy Molecule. J. Phys. Chem. 1996, 100, 19840-19846.

46. Korkin, A.A.; Bartlett, R.J. Theoretical Prediction of 2,4,6-Trinitro-1,3,5-Triazine (TNTA). A New, Powerful, High Energy Density Material? J. Am. Chem. Soc. 1996, 118, 12244-12245.

47. Korkin, A.A.; Lowrey, A.; Leszczynski, J.; Lempert, D.B.; Bartlett, R.J. Theoretical ab initio Study of CN_2O_3 Structures: Prediction of New High-Energy Molecules. J. Phys. Chem. 1997, 101, 2709-2714.

48. Chernega, A.N.; Korkin, A.A.; Romanenko, V.D.; Koigan, G.N.; Marchenko, A.P. Molecular and Electronic Structure of Halogen-Substituted Phosphaalkenes. Struct. Chem. 1997, 8, 343-352.

49. Jemmis, E.D.; Subramanian, G.; Korkin, A.A.; Hofmann, M.; Schleyer, P.v.R. The Exotic Structures of $Si_2B_2H_4$. J. Phys. Chem. 1997, 101, 919-925.

50. Gorb, L.; Korkin, A.; Leszczynski, J.; Varnek, A.; Mark, F.; Schaffner, K. Theoretical ab initio and Semi-Empirical Studies of Biologically Important Di- and Oligopyrrolic Compounds. Pyrromethenone and Biliverdin. J. Mol. Struct. (Theochem) 1998, 425, 137-145.

51. Korkin, A.A.; Nooijen, M.; Bartlett, R.J.; Christe, K.O. Theoretical Study of Bicyclic Nitrogen Tetroxide Cation, NO_4^+. J. Phys. Chem. 1998, 102, 1837-1842.

52. Gorb, L.; Korkin, A.; Leszczynski, J. Post Hartree-Fock Study of Biologically Important Di- and Tripyrrolic Compounds - Active Site of Phytochrome. J. Mol. Struct. (Theochem) 1998, 454, 137-145.

53. Peterka, D.S.; Ahmed, M.; Suits, A.G.; Wilson, K.J.; Korkin, A.A.; Nooijen, M.; Bartlett, R.J. Unraveling the Mysteries of Metastable O_4*. J. Chem. Phys. 1999, 110. 6095-6099: http://leea.lbl.gov/~musa/musa%20papers/o4.pdf

54. Srinavas, G.N.; Jemmis, E.D.; Korkin, A.A.; Scheleyer, P.v.R. An ab initio study of the Diverse $Si_3H_3^+$ Isomers. J. Phys. Chem. 1999, 103, 11034-11039

55. Korkin, A.A.; Cole, J.V.; Sengupta, D.; Adams, J.B. On Mechanism of Silicon Nitride CVD from Dichlorosilane and Ammonia. J. Electrochem. Soc. 1999, 146, 4203-4212.

56. Siodmiak, M.; Frenking, G.; Korkin, A. On Mechanism of Chemical Vapor Deposition of Ta_2O_5 from TCl_5 and H_2O. An AbInitio Study of Gas Phase Reactions. Materials Science in Semiconductor Processing, 2000, 3, 65-70.

57. Bagatyr'yants, A.A.; Novoselov, K.P.; Safonov, A.A.; Savchenko, L.L.; Cole, J.V.; Korkin, A.A. Atomistic Modeling of Chemical Vapor deposition: Silicon Nitride CVD from Dichlorosilane and Ammonia. Materials Science in Semiconductor Processing, 2000, 3, 23-29.

58. Siodmiak, M.; Frenking, G.; Korkin, A. Initial Reactions in Chemical Vapor Deposition of Ta_2O_5 from TCl_5 and H_2O. An Ab Initio Study. J. Phys. Chem. 2000, 104, 1186-1195: http://library.iem.ac.ru/j-ph-ch/2000/6-10420.html

59. Siodmiak, M.; Frenking, G.; Korkin, A. Theoretical ab initio Study of $TiCl_4$ Ammonolysis: Initial reactions of TiN Chemical Vapor Deposition. J. Mol. Modeling, 2000, 6, 413-424:

http://www.springerlink.com/app/home/contribution.asp?wasp=2g271mmymm5jxtm3ng86&referrer=parent&backto=issue,2,3;journal,28,69;linkingpublicationresults,1,1

60. Liu, C.-L.; Borucki, L.J.; Merchant, T.; Stoker, M.; Korkin, A. Ab-Initio Investigation of C Incorporation Mechanisms on Si (001). Appl. Phys. Letters. 2000, 76, 885-887.

61. Liu, C.-L.; Borucki, L.J.; Merchant, T.; Stoker, M.; Korkin A. C Incorporation Mechanisms on Si(001) surface investigated by ab initio calculations. Phys Rev. B, 2000, 62, 5021-5027.

62. Korkin, A.A.; Demkov, A.A.; Tanpipat, N.; Andzelm, J. Theoretical Investigation of the Initial Reaction of the NO Decomposition on the Si (100) (2x1) Reconstructed Surface. J. Chem. Phys., 2000, 113, 8237-8248.

63. Bagatur'yants, A.A.; Novoselov, K.P.; Safonov, A.A.; Cole, J.V.; Stoker, M.; Korkin, A.A. Silicon Nitride CVD from Dichlorosilane and Ammonia: Theoretical Study of Surface Structure and Reaction Mechanism. Surface Science, 2001, 486, 213-225.

64. Umanskii, S.Ya, Novoselov, K.P.; Minushev, A.Kh.; Siodmiak, M.; Frenking, G.; Korkin, A.A. Thermodynamics and Kinetics of Initial Gas Phase Reactions in Chemical Vapor Deposition of Titanium Nitride. Theoretical Study of $TiCl_4$ Ammonolysis. J. Comput.Chem., 2001, 22, 1366-1376. http://www3.interscience.wiley.com/cgi-bin/abstract/85007038/ABSTRACT

65. Siodmiak, M.; Govind, N.; Andzelm, J.; Tanpipat, N.; Frenking, G.; Korkin A. Theoretical Study of Hydrogen Adsorption and Diffusion on TiN(100) Surface. Physica Status Solidi (b). 2001, 226, 29-36.

66. Bersuker, G.; Korkin, A.; Jeon, Yo.; Huff, H.R. A Model For Gate Oxide Wear-Out Based On Electron Capture By Localized States. Appl. Phys. Lett. 2002, 80, 832-834.

67. Korkin, A.A.; Bersuker, G.I.; Huff, H.R. Atomistic Model of Electric Stress Induced Defect Generation in Silicon Oxide. Comput. Materials Science, 2002, 24, 223-228.

68. Knizhnik, A.A.; Bagaturyants, A.A.; Belov, I.V.; Potapkin, B.V.; Korkin, A.A. An Integrated Kinetic Monte Carlo – Molecular Dynamics Approach for Film Growth Modelling and Simulation on Si(100) Surface. Comput. Materials Science, 2002, 24, 128-132.

69. Brodskii, V.; Rykova, E.; Bagatur'yants, A.A.; Korkin, A.A. Modeling of ZrO_2 Deposition from $ZrCl_4$ and H_2O on the Si(100) Surface: Initial Reactions and Surface Structures. Comput. Materials Science, 2002, 24, 278-283

70. Novoselov, K.P.; Shirabaikin, D.B.; Umanskii, S.Yu.;Vladimirov, A.S.; Minushev, A.K.; Korkin, A.A. CHIMERA: a Software Tool for Reaction Rate Calculations and Kinetics and Thermodynamics Analysis. J. Comput. Chem. 2002, 23, 1375-1389.

71. Safonov, A. A.; Bagatur'yants, A.A.; Korkin, A.A. Oxygen Vacancies in Tetragonal ZrO_2: Ab Initio Embedded Cluster Calculations. Microelectronic Engineering, 2003, 69, 629-632.

72. Iskandarova I.M.; Knizhnik, A.A.; Rykova, E.A.; Bagatur'yants, A.A.; Potapkin, B.V.; Korkin, A.A. First-Principle Investigation of the Hydroxylation of Zirconia and Hafnia Surfaces. Microelectronic Engineering, 2003, 69, 587-593.

73. Fonseca, L.R.C.; Korkin, A.; Demkov, A.; Zhang, X.; Knizhnik, A. Atomistic Calculation of Leakage Current through Ultra-Thin Metal-Oxide Barriers. Microelectronic Engineering, 2003, 69, 130-137.

74. Bersuker, G.; Korkin, A.; Fonseca, L.; Safonov, A.; Bagatur'yants, A.; Huff, H. The Role of Localized States in the Degradation of Thin Gate Oxides. Microelectronic Engineering, 2003, 118-129.

75. Timoshkin, A.Yu.; Siodmiak, M.; Korkin, A.A.; Frenking, G. Formation of Oligomer Species in the Course of the $TiCl_4$ Ammonolysis and Their Role in Ti(IV)-T(III) Reduction Processes: A Theoretical Studies. Computational Materials Science, 2003, 27, 109-116.

76. Selezenev, A.A.; Aleynikov, A. Yu.; Gantchuk, N.S.; Yermakov, P.V.; Labanowski, J. K.; Korkin A.A. Sage MD: Molecular Dynamics Software Package to Study Properties of Materials with Different Models for Interatomic Interactions. Computational Materials Science, 2003, 28, 107-124.

77. Deminsky, M.; Knizhnik, A.; Belov, I.; Umanskii, S.; Rykova, E.; Bagatur'yants, A.; Potapkin, B.; Stoker, M.; Korkin, A. Mechanism and Kinetics of Thin Zirconium and Hafnium Oxide Film Growth in an ALD Reactor. Surface Science, 2004, 549, 67-86.

78. Bazhanov, D.I.; Knizhnik, A.A.; Safonov, A.A.; Bagatur'yants, A.A.; Stoker, M.W.; Korkin, A.A. Structure and Electronic Properties of Zirconium and Hafnium Nitrides and Oxynitrides, J. Appl. Phys. 2005, 97, 044108.

79. Novoselov, K.P.; Shirabaikin, D.B.; Umanskii, S.Yu.;Vladimirov, A.S.; Minushev, A.K.; Korkin, A.A. CHIMERA: a Software Tool for Reaction Rate Calculations and Kinetics and Thermodynamics Analysis. J. Comput. Chem. 2002, 23, 1375-1389.

80. Korkin, A.A.; Greer, J.; Bersuker, G.; Karasiev, V.; Bartlett, R.J. Computational Design of Si/SiO_2 Interface: Stress and Strain at Atomic Scale, Phys. Rev. B. 2006, 73, 165312.

81. Korkin, A.A.; Kamisaka, H.; Yamashita, K.; Safonov, A.; Bagatur'yants, A. Computational DFT Study of $ZrSiO_4$ polymorphs. Appl. Phys. Lett. 2006, 88, 181913.

82. Bartlett, R.; Karasev, V.; Greer, J.C.; Henderson, T.M.; Bersuker, G.; Korkin, A, Computational Design of Silicon Suboxides : Chemical and Mechanical Forces on the Atomic Scale, Journal of Computer-Aided Materials Design, 2006, 13, 185-200 http://www.springerlink.com/(zqbmrg3hmaehunestooikf45)/app/home/contribution.asp?referrer=parent&backto=issue,3,7;journal,1,30;linkingpublicationresults,1:102927,1

83. Greer, J.C.; Henderson, T.M.; Bersuker, G.; Bartlett R.J.; Korkin, A. Oxygen Vacancies at Si(001)/SiO2 Interface. Electrochemical Society Transactions, 2006, 2, 205-211.

84. G. Giorgi, A. Korkin, K. Yamashita, Zirconium and Hafnium Oxide Interface with Silicon: Computational Study of Stress and Strain Effects, Comp. Mat. Sci. 2008, 43, 930-937.

85. G. Giorgi, M. van Schilfgaarde, A. Korkin, K. Yamashita, On the chemical origin of the gap bowing in (GaAs)1□xGe2x alloys: a combined DFT–QSGW study, Nano Research Letters, 2010, 5, 469-477.