CURRICULUM VITAE

Voichita Maria Dadarlat
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EDUCATION:
• Ph.D. in Physics, Purdue University, May 1997. Thesis Title: "Normal Mode Calculation for Triple Helical DNA, Stability and Hydration Effects". Advisors: Lonnie Lee Van Zandt and Ronald Reifenberger.
• M.S. in Physics, Purdue University, May 1994.
• Diploma of Specialization (M.S.) in Polymer's Physics, University of Bucharest, Romania, June 1985. Thesis title: "Correlation Functions for Polymeric Systems".
• B. S. in Physics, Honors Diploma, Babes-Bolyai University of Cluj-Napoca, Romania, 1984. Thesis title: "Energy Bands and Shape Factors for Titanium".

HONORS:
• Sloan/DOE Postdoctoral Fellowship in Computational Biology, 1998-2000, Purdue University.
• Puskas Memorial Fellowship, 1994-1995, Purdue University.
• National Merit Scholarship, 1983-1984, University of Cluj-Napoca, Romania.

POSITIONS:
• Assistant Vice President for Research Compliance, Office of the Vice President for Research, Purdue University, Oct 2007 -.
• Research Security and Conflict of Interest Administrator Purdue University, Office of the Vice President for Research, Office of Research Administration, June 2006 - Oct 2007.
• Senior Research Scientist, Purdue University, Departments of Computer Science and Medicinal Chemistry and Molecular Pharmacology, July 2005 -June 2006.
• Research Scientist, Purdue University, Department Medicinal Chemistry and Molecular Pharmacology, July 2005 - . Advisor: Carol Post.
• Assistant Research Scientist in Theoretical Physical Chemistry, Purdue University, Department of Chemistry, August 2001 - June 2005.
• Visiting Postdoctoral Fellow at Lawrence Berkeley Laboratories, Physical Biosciences Division, August 2000-June 2001. Advisor: Teresa Head-Gordon.
• Tenure Track Assistant Professor offer in the Department of Physics at Wake Forest University, Winston-Salem NC, April 2001, *declined.*
• Tenure Track Assistant Professor offer in the Department of Physics at Marquette University, Milwaukee, WI, March 2001, *declined.*
• Sloan/DOE Postdoctoral Fellow in Computational Molecular Biology, Purdue University, Department of Medicinal Chemistry and Molecular Pharmacology (1998-2000).
• Postdoctoral Research Associate, Purdue University, Department of Medicinal Chemistry

and Molecular Pharmacology (1997-1998).
- Teaching and Research Assistant, Purdue University, Department of Physics (1992-1997).
- Researcher, Research Institute for Plastic Materials, Bucharest, Romania (1985-91).
- High School Teacher and Junior Physicist at Ploiesti Petrochemical, Romania (1985-1987).

RESEARCH INTERESTS:

My research interests are in Computational Biology and Biophysics:
- Modulation of DNA Transcription by Activator–Coactivator Complexes: pKID-KIX and cMyb-KIX, genetic medication;
- Potentials of Mean Force and the Free Energy of Protein–Ligand Binding;
- Applications of PMFs and Free Energy of Binding Methods to Biosensor Design;
- Protein–Protein and Protein–Solvent Interactions;
- Protein Folding and Stability as it relates to monogenic deseases and SNPs;
- Protein Thermodynamics and Protein Structure Prediction;
- DNA Electrodynamics.

PUBLICATIONS:

1. V. M. Dadarlat and R. Skeel. "Absolute Free Energy of Binding for the DNA Activator/Coactivator Complexes of KID-KIX and pKID-KIX." Biophys. J. (2011) 100:469-477.

2. V. M. Dadarlat and C. B. Post . "Contribution of Charged Groups to the Enthalpic Stabilization of the Folded States of Globular Proteins". J. Phys. Chem. B (2008) 112(91):6159-6167.

3. V. M. Dadarlat and C. B. Post. Decomposition of Protein Experimental Compressibility into Intrinsic and Hydration Shell Contributions Biophys. J. (2006) 91:4544-4554.

4. V. M. Dadarlat. "Potentials of mean force (PMFs) for the interaction of blocked alanine dipeptide molecules in water and gas phase from MD simulations". Biophys. J. 2005, 89: 1433-1445.

5. V. M. Dadarlat and C. B. Post. "Adhesive-cohesive model for protein compressibility: an alternative perspective on stability". Proc. Natl. Acad. Sci., U.S.A. (2003) 100(25): 14778-14783.

6. V. M. Dadarlat*, S. Zhong*, T. Head-Gordon, R. M. Glaeser and K. Downing. "Modeling Chemical Bonding Effects for Protein Electron Crystallography: the transferable fragmental electrostatic potential (TFESP) method". Acta Cryst. A 58: 162-170, Part 2, 2002. $*^{Equal Authorship}$.

7. V. M. Dadarlat and C. B. Post. "Insights into Protein Compressibility from Molecular Dynamics Simulations". Journal of Physical Chemistry, 105(3):715-724, 2001.

8. C. B. Post and V. M. Dadarlat. "Molecular Dynamics Simulations of Biological Macromolecules." International Tables for Macromolecular Crystallography. Vol F. (2000) M. B. Rossman and E. Arnold, eds. Kluwer Academic Publishers, London.

9. V. M. Dadarlat and V. K. Saxena. "The Effect of Structural water Molecules on the Normal mode Spectrum of $dT_n \cdot dA_n \times dT_n$ DNA". J. Biomol. Struc. Dyn., 17(2):333-346, 1999.

10. V. M. Dadarlat and V. K. Saxena. "Stability of Triple helical Poly(dT)-Poly(dA)-Poly(dT) DNA with Counterions". Biophys. J., 75:70-91, 1998.

11. V. M. Dadarlat, V. K. Saxena and L. L. Van Zandt. "Semiclassical IR/Raman Spectroscopy of DNA Polymer". J. Biomol. Struc. Dyn. 12, a041 (1995).

12. V. M. Dadarlat, I. Deaconescu and M. Georgescu. "The characterization of Styrene-acrylonitrile copolymer by ultracentrifugation". Plastic Materials, No. 1 (1990), p.33-37.

13. V. M. Dadarlat, Lev Gorenstein and C. B. Post. "Global Prediction of wild type and mutated proteins enthalpic stability from MD simulations of proteins and peptides", In preparation.

EXPERTISE:
Experimental: Physical characterization of Polymers and Copolymers through ultracentrifugation and chromatography.
Computer expertise: CHARMM, VMD, QUANTA, Q-CHEM, UNIX platforms, Scientific Fortran programming, Shell Scripting, Matlab, Mathematica, COEUS.
Application for research funding (to NIH and NSF). Proposal title: "Potentials of mean force for protein-protein interactions". This research aims to develop a good methodology for calculating the free energy of protein–ligand binding and understanding the specific contributions from ligand phosphorylation for protein–ligand complexes involved in DNA transcription: the pKID-KIX and the cMyb-KIX complexes. *Not funded.*
Research Administration:
• Application and implementation of federal regulations, state statues and university policies to the university research compliance programs.
• Management of Financial Conflicts of Interest for all Purdue Employees, Human Research Protection, Export Control Programs;
• Responsible Conduct of Research, Ethical Issues in Research with Human Subjects;
• Work with Faculty, Staff, Students, Department Heads and Deans, the Provost's and Treasurer's Offices, Sponsored Program Services, Purchasing Services, College and Departmental Business Offices, Office of Technology Commercialization and Purdue Research Foundation, other offices within the Office of the Vice President for Research.

TALKS and PRESENTATIONS:
a. Research Presentations:
• "A Recipe for predicting amino acid enthalpy contributions to protein folded state stability - wild type and mutants", Purdue NMR Symposium, May 11th, 2010.
• "Application of the restraining potential method for binding energies", Mathematical and Numerical Methods for Free Energy Calculations, Molecular Systems workshop at the Banff International Research Station for Mathematical Innovation and Discovery, June 15 - 20, 2008 (presenter Robert Skeel).

- "Potentials of Mean Force and Free Energy of Binding for Protein–Protein and Protein–Ligand interactions" - talk presented at the Computing Research Institute Seminar, Dept. of Computer Science, Purdue University, April 5th, 2006.
- "Computational Studies of Protein Stability and Protein–Protein Interactions" - talk presented at the Physical Chemistry Seminar, Dept. of Chemistry, Purdue University, Sept. 21st, 2005.
- "Solute-Solute Potentials of Mean Force and Time Correlation Functions for the Interaction of Two Blocked Alanine Dipeptide Molecules" - talk presented at the Midwest Thermodynamics Conference, Purdue University, May 2005.
- "Towards potentials of mean force for protein-protein interaction: the case of alanine dipeptide"- poster presented at the AM-3 Conference for Molecular Modeling, University of Leicester, UK, August 2004.
- "Modeling Chemical Bonding Effects for Protein Electron Crystallography". Teresa Head-Gordon, Dept. of Bioengineering, University of California, Berkeley, Voichita M. Dadarlat, Dept. of Chemistry, Purdue University, West Layfayette, IN, et al., Electron Microscopy of Biological Macromolecules-II, Invited talk, San Antonio TX, 2002.
- "Isothermal compressibility of globular proteins", Department of Physics, Purdue University, West Lafayette IN, April 2001.
- "Compressibility, Intraprotein and protein-water interaction in globular proteins", Department of Physics, Wake Forest University, Winston-Salem NC, April 2001 (tenure track offer, April 2001).
- "Compressibility and protein Matrix Entropy in Globular Proteins", University of California, Northridge, March 2001.
- "Isothermal compressibility of globular proteins" Marquette University, Milwaukee, WI, February 2001 (tenure track offer, March 2001).
- "Intraprotein and protein-water interaction in globular proteins", Lawrence Berkeley Laboratories, July 2000, Berkeley, CA.
- "Configurational Entropy, Compressibility and Packing Density in Globular Proteins", APS March Meeting, March 20-24, 2000, Minneapolis, MN.
- "What Physicists can do for Biology in the Post-Genomic Sequence Era", Purdue Univ., Physics Dept., February 8, 2000.
- "Compressibility, Entropy and Internal Energy Partitioning in Globular Proteins", poster presented at the Quantitative Challenges in the Post-Genomic Sequence Era Meeting, January 11-15, 2000, San Diego, CA.
- "Intrinsic compressibility and configurational entropy: possible implications in protein structure prediction and stability", Structural Biology Seminar, October 13, 1999, Purdue University, West Lafayette, Indiana.
- "Exploring the Protein PVT Conformational Space Through Isothermal Compressibility Calculation", First annual DOE Computational Structural Biology Research Meeting, December 18-19, 1998, Monterey, California.
- "Is there a Linear Relationship between Thermal Stability and Compressibility for Globular Proteins?" V. M. Dadarlat and C. B. Post, poster presented at the Structure-Based Functional Genomics Meeting, October 4-7, 1998, Avalon, NJ.
- "Normal Modes in Triple-Helical poly(dT)-poly(dA)-poly(dT) DNA Structure", APS March Meeting, 18-22 March 1996, St. Louis, Missouri.

b. Research Administartion Presentations:

• "Conflicts of Interest in IRB Protocol Reviews". A Presentation for Social Sciences Institutional Review Board Members at Purdue University, Sept. 28th, 2010.

• "The Good (Senator?), The Bad (Researcher?), and The Ugly (Consequences);A tale of Conflicts of Interest, Consequences, and Lessons Learned". Purdue University, Sponsored Programs Services - Seminar Series, March 5th, 2009.

• "From Student Academic Integrity to the Responsible Conduct of Research; A primer for future academic and civic leaders." Purdue Student Leadership Seminar Series, April 9th, 2009.

• "Outside Activities and the Enigmatic Form 32A", a presentation for future entrepreneurs. Purdue May 19th, 2009.

• "Conflicts of Interest in IRB Protocol Reviews". A Presentation for Biomedical IRB Members at Purdue University, Oct. 19th, 2010.

ACCOMPLISHMENTS

Top ten accomplishments as an Assistant Vice President for Research:

1. Designed and, in collaboration with SPS, implemented the university compliance program with PHS/NIH regulations regarding research objectivity - the management and reporting of Conflicts of Interest in research, including the addition of regulatory review for disclosed financial interests in COEUS; redesigned the pdf interactive Financial Interest Statement form, the C-1 Form, and the COI Management plans. **2.** Completed the restructuring and reorganization of electronic record-keeping of documents for all COI related records. Improved the capabilities of our database by adding specific SQL inquiries and new linked tables such as contact information for employees, Oversight Managers, Department Heads, Deans, and DFAs. **3.** Designed the ORA Conflict of Interest (COI) and Export Control (EC) websites and contributed most of the content for the COI website and content for the EC website (e.g. Investigator Responsibilities). **4.** Reformatted previously paper-based Forms 32A, 35, C-1 in electronic pdf interactive format and made them available on the web for easy access and completion. **5.** Redesigned the COI Annual Review process. Renewal packages for applications for permission to engage in outside activities are now sent to employees and their Oversight Managers in all electronic, pdf interactive format, compacted into .zip files containing applicable 32A, 35 and C-1 Forms, and customized Annual Reports. These procedures lead to a noticeable improvement in the timely resubmission of applications for permission to engage in outside activities and saved time, money, and employee effort. **6.** Routinely prepare summaries and submit Financial Interest disclosures (Forms C-1) to the Board of Trustees for all Purdue Employees on behalf of the Office of Research Administration. **7.** Have served as the leading person from Purdue for testing the Conflict of Interest Module in COEUS Lite, an investigator focused interface of COUES that allows for collaboration in Proposal Development, and on time completion/submission of compliance-driven applications related to Human Subjects Research and COI/Financial Interest disclosures. **8.** Prepared and presented to the COEUS Compliance Subcommittee reports on the status of the COI Module and its functional deficiencies. **9.** Designed a comprehensive algorithm/ process description for event - driven COI disclosure of SFI that meets the requirements of PHS/NSF regulations at the time of proposal submission; the same process can be imple-

mented for financial interest disclosure in IRB application for engagement in Human Subjects Research. **10.** This algorithm will be implemented in COEUS Lite by the COEUS Development team at MIT.

SERVICE

I am a member of, and have contributed to the work of several university committees:
o Hazards Management Oversight Committee **o** Data Stewardship Committee **o** IRB Social Sciences Committee **o** IRB Biological Sciences Committee o IRB Executive Committee **o** COI working groups at OVPR and the Provost's Business Office **o** Export Control/Research Security Committee **o** Computational Social Science Task Force Committee **o** Cloud Computing Committee **o** OVPR website development Committee, and **o** the multi-institutional COEUS Compliance Committee.

PROFESSIONAL ACTIVITIES:

Reviewer for the Biophysical Journal
Reviewer for Protein Science
Reviewer for J. Chem. Phys.
Reviewer for Nucleic Acids Research
Mentor for MARC/AIM Summer Research Program for Undergraduates, 2002
Member of the APS, 1997-2004.

LANGUAGES:

English (fluent),
Romanian (fluent),
French (good working knowledge).