

FELICIA PITICI

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Education	MOUNT SINAI SCHOOL OF MEDICINE OF NEW YORK UNIVERSITY New York Ph. D. in biophysics, August 1999 Emphasis on computational methods of molecular modeling, molecular dynamics simulations, vibrational analysis, Green's function analysis GPA 3.67/4.00
	THE INTERNATIONAL CENTER OF THEORETICAL PHYSICS Trieste, Italy Pre-doctoral workshop in physics, August-September 1991 Emphasis on statistical physics and quantum mechanics
	UNIVERSITY OF BUCHAREST Bucharest, Romania Honors degree with distinction in physics, June 1988 M. S. in physics, June 1987 Emphasis on solid-state physics, statistical physics, quantum mechanics Final course grade and theses evaluations: 10; 10/10
Experience 2003-	WESLEYAN UNIVERSITY Middletown Visiting assistant professor <ul style="list-style-type: none">• Develop curriculum of applications of physics to biological systems• Teach the Introductory Physics course
1999-2002	WESLEYAN UNIVERSITY Middletown Research associate ; Visiting assistant professor <ul style="list-style-type: none">• Performed computational studies of nucleic acids and protein-RNA systems and investigated the relationship to biological functions• Taught computational biophysics and experimental optics
1992-1999	MOUNT SINAI SCHOOL OF MEDICINE OF NEW YORK UNIVERSITY New York Ph. D. Thesis Research <ul style="list-style-type: none">• Characterized computationally the structure-function relationship for EF-hand calcium-binding proteins• Taught physics to MCAT candidates
1990-1992	UNIVERSITY OF BUCHAREST Bucharest, Romania Assistant professor; Private tutor <ul style="list-style-type: none">• Taught statistical physics, molecular physics, mechanics• Conducted laboratory experiments in molecular physics and mechanics
1988-1990	INSTITUTE FOR NUCLEAR POWER REACTORS Pitesti, Romania Physicist <ul style="list-style-type: none">• Performed theoretical and computational studies of nuclear fuel materials• Conducted physical and chemical tests of materials for nuclear fuel ensembles

- Skills**
- Experience with computational methods of sequence analysis, molecular modeling, free energy calculations, vibrational analysis, Green's function analysis
 - Experience with techniques of molecular dynamics, Brownian dynamics, Monte Carlo simulations, stochastic path integration
 - Practice with the computational chemistry software CHARMM, AMBER, GROMOS, MOIL, MACROMODEL, GAUSSIAN
 - Familiar with the molecular visualization software INSIGHT, QUANTA, GRASP, VMD, MIDAS
 - Computer literacy: UNIX, MacOS, Windows; Programming language: FORTRAN
- Publications**
- Felicia Pitici (2003). Structural Preference for Changes in the Direction of the Ca²⁺-Induced Transition: a Study of the Regulatory Domain of Skeletal Troponin-C, *Biophysical Journal* **84**:82-101 (Journal Cover Illustration)
 - Felicia Pitici, Anne Baranger, and David L. Beveridge (2002). Computational Studies of Induced Fit in U1A-RNA Interaction: Do Molecular Substates Code for Specificity?, *Biopolymers* **65**:424-435
 - Felicia Pitici and David L. Beveridge (submitted). A-Tract DNA Bending Revisited: Comparative Analysis of Molecular Dynamics Simulations and Experiment, *Journal of Molecular Biology*
 - Felicia Pitici (submitted). Invited Review: Determinants for Protein-RNA Binding: Studies of the RNA-Recognition Motif U1A and of Target RNAs, *Cell Biochemistry and Biophysics*
 - Willy Wriggers, Ernest Mehler, Felicia Pitici, Harel Weinstein, and Klaus Schulten (1998). Structure and Dynamics of Calmodulin in Solution, *Biophysical Journal* **74**:1622-1639 (Journal Cover Illustration)
 - Felicia Pitici and Speranta Svirschevski (1991). Effective Phonon Theory for DNA Melting, *Physical Review* **44A**:8348-8355
 - Felicia Pitici (1991). Problems Concerning Some Periodical Motions, *Romanian Journal of Physics* **4**:38-41
 - Felicia Pitici (1988). Hidden Parameters Theories in the Interpretation of Quantum Mechanics, in *National Colloquy: History and Philosophy of Sciences* **2**:955-964, University of Iasi Press, Romania
 - Felicia Pitici (1989-1991). Original problems proposed for college and high-school students, *Romanian Journal of Physics and Chemistry*
- In preparation**
- Felicia Pitici and David L. Beveridge. Molecular Mechanisms for Structural Adaptation in U1A-RNA Interaction, *Journal of the American Chemical Society*
 - Felicia Pitici and David L. Beveridge. Energetics of Binding the Spliceosomal U1A Protein to Hairpin RNA: a Free Energy Decomposition Analysis, *Biophysical Journal*
 - Felicia Pitici. A Predictor of Activity in Calmodulin Structural Congeners: the Propensity for Helix-Coil Structure in the Linker Residues 77-81, *Cell Biochemistry and Biophysics*
- Abstracts**
- Felicia Pitici (2001). Ca²⁺-Sensing Mechanisms in Calmodulin and Troponin-C, *Biophysical Journal* **80**:A397
 - Felicia Pitici and David L. Beveridge (2001). U1A: Structural and Dynamic Determinants for Function, *Biophysical Journal* **80**:A2568
 - Felicia Pitici and David L. Beveridge (2001). Determinants for specificity in U1A-RNA interaction, *Journal of Biomolecular Structure and Dynamics* **18**:974
 - Felicia Pitici and Harel Weinstein (1999). Structural and Dynamic Determinants for Ca²⁺-Dependent Properties of Skeletal and Cardiac Troponin-C, *Biophysical Journal* **76**:A275
 - Felicia Pitici, Chung F. Wong, and Harel Weinstein (1998). A Predictor of Activity in Calmodulin Structural Congeners: the Propensity for Helix-Coil Structure in the Linker Residues 77-81, *Biophysical Journal* **74**:A348
 - Felicia Pitici, Ernest Mehler, and Harel Weinstein (1996). Molecular Dynamics at a Target Binding Surface of Calmodulin, *Biophysical Journal* **70**:A48
 - Felicia Pitici, Ernest Mehler, and Harel Weinstein (1994). Structural Dynamics of TnC Mutants with CaM-like Properties, *Biophysical Journal* **66**:A71
 - Felicia Pitici and Speranta Svirschevski (1990). Model for DNA Melting, Volume of the International Meeting in Biochemistry and Biophysics, Romania

- Courses, Presentations
- Invited Lecturer. Introductory Physics, Wesleyan University, USA (currently)
 - Invited Speaker. Across Length and Time Scales: Newton's Second Law of Dynamics, University of Maine, Orono, USA (2003)
 - Invited Speaker. Energetics of Binding the Spliceosomal U1A Protein to Hairpin RNA: a Free Energy Decomposition Analysis, Yale University, USA (2003)
 - Invited Speaker. Computational Studies in Molecular Biophysics: the Mechanisms for Function in Protein-RNA Interaction, Harvard University, USA (2002)
 - Invited Speaker. Molecular Mechanisms for Structural Adaptation in U1A-RNA Interaction, Swiss Federal Institute of Technology, Switzerland (2002)
 - Platform Presenter. Nano Ca^{2+} -Sensors of Biological Function, American Physical Society Meeting, New England Section, USA (2002)
 - Invited Lecturer. Experimental Optics, Wesleyan University, USA (September-December 2001)
 - Invited Lecturer. Advanced Topics in Computational Biophysics, Wesleyan University, USA (February-May 2001)
 - Invited Speaker. Ca^{2+} -Sensing Mechanisms in Calmodulin and Troponin-C, International Workshop on New Biophysical Methods in Biology and Medicine, Romania (2000)
 - Invited Speaker. Molecular Mechanisms for Function in Biological Ca^{2+} -Sensors, University of Bucharest, Romania (2000)
 - Platform Presenter. Structural and Dynamic Determinants for Ca^{2+} -Dependent Properties of Skeletal and Cardiac Troponin-C, Biophysical Society Meeting, USA (1999)
- Meetings, Workshops
- American Physical Society Meeting, New England Section, USA (2002)
 - 12th Conversation in Biomolecular Stereodynamics, USA (2001)
 - NIH Workshop in Computational Biology Tools, USA (2000)
 - International Workshop on New Biophysical Methods in Biology and Medicine, Romania (2000)
 - Biophysical Society Meeting, USA (1994-2001)
 - International Symposium on Calcium-Binding Proteins, USA (1995)
 - Workshop in Theoretical Chemistry: *ab initio* Methods, USA (1993)
 - International Meeting in Biochemistry and Biophysics, Romania (1990)
 - National Colloquy of History and Philosophy of Sciences, Romania (1988, 1986)
- Awards
- First award at the National Student Meeting in Physics, Romania, 1987
 - Awards at the National Olympiads of Physics, Romania, 1981-1983
- Research
- Proposed a novel principle by which RNA-binding proteins select their targets
 - Applied a free energy decomposition scheme to identify the contributions to binding the spliceosomal U1A protein to cognate RNA sequences
 - Proposed criteria for convergence of the free energy components from molecular dynamics simulations
 - Studied the structural, dynamic, and energetic properties of four U1A-derived constructs with altered RNA-binding affinity, and of the corresponding U1A-RNA complexes
 - Used Monte Carlo algorithms to characterize the structural preference of the C-terminal region of U1A, a critical element for recognition in U1A-RNA interaction
 - Performed molecular dynamics simulations to assess the structure and dynamics of A-T rich DNA sequences, and to compare the results with NMR and X-ray data
 - Showed that simulation protocols can correct the DNA-bend of crystal dodecamers to the direction observed in solution preparations
 - Proposed an approach for calibrating parameters in molecular dynamics and GBSA simulations of nucleic acids, and in prediction algorithms using dinucleotide models
 - Adapted FORTRAN programs for Brownian dynamics simulations of nucleic acids
 - Performed statistical analysis of nucleic acids parameters from the NDB server
 - Proposed a novel view of the Ca^{2+} -induced transition in modulatory proteins of the EF-hand family, and emphasized applications to Ca^{2+} -sensing molecular devices

- Analyzed the harmonic and quasiharmonic vibrational modes of individual globular domains of skeletal and cardiac troponin-C (TnC), and of calmodulin (CaM)
- Performed Green's function analyses to characterize the structural response of EF-hand domains to perturbations produced upon binding/releasing Ca^{2+}
- Identified the reaction path for the apo→holo transition of the regulatory N-terminal domain of skeletal TnC
- Performed Green's function analyses to identify elements critical for the equilibrium between apo and holo states of the N-terminal domain of CaM, and estimated free energy changes to small variations of the atomic parameters
- Applied a variational method to estimate pK values for the regulatory N-terminal domains of skeletal and cardiac TnC, and proposed a functional role for the observed differences
- Applied a recently proposed helix-coil theory to CaM, skeletal and cardiac TnC to assess the helical propensity of the linker between globular domains in relationship to the observed phenotype
- Performed molecular dynamics simulations of CaM, skeletal TnC, skeletal TnC-derived mutants, and of individual EF-hand domains using various solvation models
- Characterized the conformation of a six residue-long segment at the N-terminus of CaM using simulated annealing and Monte Carlo sampling
- Wrote programs to analyze the correlations between internal motions for various molecular systems, e. g. dipeptides, BPTI, cytochrome-C, the C-terminal domain of CaM
- Developed an effective phonon theory to model DNA denaturation, and derived analytical expressions for the thermodynamic properties characteristic of the transition
- Performed time-resolved fluorometry to characterize collective motions in biological membranes, and proposed a model for studying the kinetics of monomer-excimer reactions

REFERENCES – Felicia Pitici

- Professor Harel Weinstein, Chair
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