Molecular Biophysics

Prof. Thomas Kurtzman, Subdiscipline Chair
simpleliquid@gmail.com

Publications


Research Areas

- Biophysical mechanisms of ligand binding
- Structural Biology
- Neutron scattering
- X-ray Crystallography
- Protein NMR
- Computational biophysical chemistry
- Enzymology
- Biotechnology

Protein–RNA interactions in the human spliceosome revealed by Prof. Nancy Greenbaum (Hunter College)

ssNMR studies of plant-based polymer feedstocks by Prof. Stark (City College)

Bioinformatics of Light–Oxygen–Voltage photoreceptors by Prof. Gardner (Advanced Science Research Center)
Name: Zimei Bu  
Position: Professor  
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Dr. Bu's group studies the structure and dynamics of protein complexes in cell signaling, using neutron and X-ray scattering.

2010- current  Professor, CCNY  
2003-2010  Faculty, Fox Chase Cancer Center  
1999-2002  Chemist, NIST  
1994-1999  Postdoc, Yale University  
1994  PhD, Louisiana State University

Research Interests

• Keywords: Biophysics; Cell Signaling; Structure; Dynamics; Kinetics; Molecular Recognition; X-ray Scattering; Neutron Scattering

Our group studies the structure and dynamics of cell signaling proteins and macromolecular complexes that regulate cell adhesion, and the intracellular trafficking of membrane receptors and ion channels. These proteins function as molecular machines and switches that can fail to work properly for various reasons, causing diseases such as cancer. We employ biochemical, biophysical, and structural biology techniques, in particular small angle neutron and x-ray scattering (SAXS and SANS), to study the interactions of these proteins. We also develop methods of utilizing quasielastic neutron scattering, in particular neutron spin echo spectroscopy (NSE) to study protein dynamics and protein domain motions. We have developed a theoretical framework using non-equilibrium statistical mechanics to interpret the NSE data. These methods allow us to see, for the first time, the dynamics of protein complexes on nanometer scales. NSE fills an important information gap in our ability to study protein motion on sub-microsecond time scales and on nanometer length scales.

Publications


Dr. Junyong Choi

Junyong Choi is a synthetic and computational medicinal chemist. His research focuses on development of therapeutic candidates by applying organic synthesis, computer-aided drug design, and chemical biology.

Research Interests

Keywords: Medicinal Chemistry, Organic Synthesis, Computer-aided Drug Design, Chemical Biology

My scientific objective is to develop specific, target-directed therapeutic candidates for human diseases. My laboratory integrates organic synthesis, medicinal chemistry, computer-aided drug design, and chemical biology to discover bioactive chemical probes. We are particularly interested in discovery of small molecule agents with novel mechanism of action to elucidate specific functions of biological targets. The discovery and techniques established in my laboratory will advance the chemical science in biomedical research for the development of therapeutics.

Publications

JY Choi, et. al., Comparative structural analysis and molecular design for the development of highly potent and selective agents targeting Matrix Metalloproteinase 13, *J. Med. Chem.*, **2017**, 60, 5816-5825


The overarching goal of the Deri Lab is the integration and application of radiochemistry towards tangible benefits to society. We focus on the intersection of radiochemistry and biomedical science, more specifically in molecular imaging and radiotherapy using radioactive metals.

Research Interests

Keywords: Radiochemistry, Radiopharmaceuticals, Nuclear Medicine, Radiometals, Chelators, Chemical Education, Pedagogy

Prof. Deri’s research efforts are focused on addressing the following two questions:

How can radioactivity be used to improve human health? Research projects include:
- Radiometal chelation studies
- Bifunctional chelator development
- Radiopharmaceutical design

How can we get more people interested in chemistry? Teaching practices and strategies studied:
- Culturally relevant teaching practices
- Use of technology in education
- Online learning tools
- Flipped classroom pedagogy
- Active learning strategies

Publications


Dr. Ruel Desamero is a spectroscopist by training currently investigating protein-ligand interaction as well as protein-protein aggregation using various techniques.


Research Interests

Keywords: vibrational spectroscopy; fluorescence; circular dichroism; temperature-jump techniques; structural biology; protein biochemistry; enzymology

My research is centered on investigating the structural and dynamical aspects of protein-small molecule interactions using techniques such as vibrational spectroscopy and temperature-jump relaxation. One aspect of the work is to understand at the molecular level how protein systems work. Enzyme-substrate interactions have long been recognized as representing an extreme expression of structural complementarities in biological chemistry. Basic research geared towards understanding the inner workings of an enzyme system is important if cures for the diseases caused by a malfunctioning or deficient enzyme are to be found. We have also started investigating the mechanism behind amyloid formation with the goal of synthesizing peptide inhibitors that diminish protein aggregation.
Amedee des Georges
Assistant Professor, ASRC Structural Biology Initiative
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2015- current
Assistant professor, Structural Biology Initiative, CUNY Advanced Science Research Center
Assistant professor, Department of Chemistry and Biochemistry, City College of New York

2008-2015
Postdoc – HHMI / Columbia University – (w/ Dr. Joachim Frank)

2004-2008
PhD – MRC-Laboratory of Molecular Biology, Cambridge, UK – (w/ Drs. Linda Amos & Jan Lowe)

Research Interests

Keywords:
Cell regulation • Cancer • Heart diseases • Biochemistry • Molecular biology • Structural biology • Cryo-electron microscopy • Image analysis • Modeling • Methods development • Translation initiation • Membrane proteins • Calcium signaling

Publications


des Georges et al., Structure of the mammalian ribosomal pre-termination complex associated with eRF1• eRF3• GDPNP, Nucleic acids research, 2013, gkt1279.

The des Georges lab is interested in the molecular mechanisms of cell regulation. We use cryo-electron microscopy to decipher at the atomic level the function of large macromolecular complexes involved in calcium signaling and in the regulation of protein synthesis.
Dr. Terry Dowd is involved in two areas of research. One area is the alteration in bone mineral properties in disease. The second project involves alterations in structure–function relationships in the gap junction molecule Connexin in deafness, neuropathy and skin disease.

My research involves investigating the role of the bone protein osteocalcin in bone mineral diseases such as Pb2+ toxicity, low Mg2+ diets and diabetes. The research involves multiple techniques such as atomic absorption, FTIR Imaging and microCT to investigate alterations in mouse bone mineral properties. The second project involves NMR structural-functional studies of the gap junction molecule Connexin in health and diseases such as deafness, fatal skin disease and neuropathy. The project uses 2D NMR techniques on a high field magnet and electrophysiological techniques characterizing the mutant gap junction channels.

Publications


Emilio Gallicchio's research is in the area of computational molecular biophysics. He uses advanced computational models to investigate the dynamics and thermodynamics of biological systems.

Dr. Emilio Gallicchio
Assistant Professor
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Publications


Research Interests

- Thermodynamics of protein-protein and protein-ligand binding
- Virtual drug screening
- Protein conformational equilibria
- Statistical thermodynamics of protein folding and misfolding
- Thermodynamics of solvation of biological macromolecules
- Force field development and high resolution protein modeling
- Design of high performance computational chemistry algorithms
- Parallel and distributed computing
Dr. Kevin H. Gardner

The Gardner lab studies how cells perceive and respond to changes in the environment around them. Such information provides insights into fundamental principles of protein structure and signaling, guides the engineering of new protein-based tools, and lays the foundation for new therapeutic strategies.

Kevin H. Gardner
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CUNY Advanced Science Research Center, Room 3.322
85 St. Nicholas Terrace
New York, NY 10031
Kevin.Gardner@asrc.cuny.edu
structbio.asrc.cuny.edu • kglab.org

Publications

Y. Guo et al., Coiled-coil coactivators play a structural role mediating interactions in hypoxia inducible factor heterodimerization. *J. Biol. Chem.*, 2015, online now.


Research Interests

Keywords: environmental sensing • protein/protein interactions • ligand binding • allostery • NMR spectroscopy • X-ray diffraction • biochemistry • photosensors • cancer • protein engineering
The Gibney Lab uses metalloprotein design to investigate the fundamental engineering of biological systems. These studies provide insight into metal-induced protein folding, heme electrochemistry, and the role of chemically modified hemes in biology.

# Publications


Gibney, B.R. Metallopeptides as Tools to Understand Metalloprotein Folding and Stability in Protein Folding and Metal Ions – Mechanisms, Biology and Disease, Gomes, C and Wittung-Stafshede, P. Eds. 2011, 227-245.

# Research Interests

**Keywords:** De novo metalloprotein design, inorganic coordination chemistry, biophysics, bioenergetics, electrochemistry

Our research focuses on the role of metal ions in biological systems from both an inorganic coordination chemistry and biophysical perspective. We are currently investigating the role of zinc in controlling gene expressions in human cancer, and the role of heme proteins in cardiovascular disease.
Dr. Dixie J. Goss

**Publications**


**Research Interests**

*Keywords: protein synthesis, virus, protein-nucleic acid interactions*

We use biophysical approaches to understand how non-coding regions of mRNA regulate function. Miss regulation of protein synthesis is responsible for many diseases including cancer. We are interested in how unique structures in viral RNA allow viruses to take over host cell protein synthesis.
Dr. Green is a computational chemist, with a principal interest in biophysical problems, especially related to a class of proteins, ion channels, responsible for the nerve impulse, among other things.

Dr. Green has been a faculty member in Chemistry at CCNY since Sept 1966.

Research Interests

Keywords: Quantum calculations, proteins, water structure, hydrogen bonds, salt bridges, membranes, water transport through membranes

Research Strategy: Primarily we carry out quantum calculations on overlapping sections of proteins, such as voltage sensing domains of ion channels, to determine structure, bonding, energetics, and transitions of protein, water, hydrogen bonds, and salt bridges, leading to mechanisms, for example, of sensing voltage.
Publications


Popović, M, Greenbaum, NL (2014) Role of helical constraints of the EBS1-IBS1 duplex of a group II intron on demarcation of the 5’ splice site. RNA 20, 24-35.


Popović, M, Nelson, JD, Schroeder, KT, Greenbaum, NL (2012) Impact of base pair identity 5’ to the spliceosomal branch site adenosine on branch site conformation. RNA 18, 2093-2103.

Research Interests

Keywords: RNA, spliceosome, NMR

We attempt to answer questions about how RNA molecules fold and interact with other RNA, metal ions, and proteins in order to carry out the complex activity of precursor messenger (pre-m)RNA splicing. This process, by which noncoding intron sequences of pre-mRNA molecules are excised and flanking coding exons are ligated together, is an essential step in preparation of mRNA transcripts prior to translation of their message into protein sequences.

Pre-mRNA splicing in eukaryotic cells is performed by the spliceosome, a dynamic nuclear supramolecular assembly that comprises five recyclable small nuclear (sn)RNA molecules and many proteins. Similarities between spliceosomal snRNAs of and functionally analogous regions of Group II introns, which excise themselves even in the absence of proteins, suggests shared evolutionary ancestry and the likelihood that the spliceosomal reaction is also catalyzed by its RNA components. Using a combination of biochemistry, biophysical, and spectroscopy techniques, we characterize the molecular basis of recognition and conformational dynamic leading RNA splicing in the two systems.
Elucidation of transition metal-mediated processes undertaken by pathogens and the corresponding immune response by the human body during infection using bioinorganic, biophysical and computational methodologies.

**Research Interests**

*Keywords:* Bioinorganic Chemistry, Spectroscopy, Biophysical Chemistry, Magnetic Resonance, Quantum Chemical Calculations

Transition metal homeostasis is one of mechanisms through which the human body combats microbial attack. We are investigating both the processes undertaken by pathogens during invasion of a host cell and the responses executed by the host cell during such an attack. The research projects aim to study the mechanisms of zinc and copper homeostasis, incorporation of native metal ions by metallochaperones, and pathogenic machinery of zinc acquisition. Investigation of these physiological events at the interface of chemistry and biology will provide atomic-level understanding of fundamental processes in the human body during microbial invasion, which will have significant implications for human health and in the design of efficient therapeutics.

**Publications**

Dr. David Jeruzalmi

Jeruzalmi’s group applies X-ray crystallography, supplemented with electron microscopy, to understand these long-standing problems in DNA biology. We also use biochemical studies to inform these approaches and follow up on the resulting insights.

Research Interests

The faithful transmission of gene1c information is an important biological imperative. To carry out this function, organisms have evolved processes to replicate their genomes and defend them from attack. We study important mechanisms associated with the processes of DNA replication and repair. The central challenge in understanding these processes stems from the large size of the involved multi-protein DNA complexes; these entities also populate many conformational states. Together, these complications place limits on insights that can be revealed by static crystallographic structures or solution methods alone; both sources of information are essential for defining underlying mechanisms. To this end, my group applies X-ray crystallography, supplemented with electron microscopy, to understand these long-standing problems in DNA biology. We also use biochemical studies to inform these approaches and follow up on the resulting insights.

Publications


Dr. Daniel A. Keedy

The Keedy Lab is interested in how atomic motions imbue protein molecules with biological functions. We use novel X-ray experiments plus computational modeling to explore dynamic processes like ligand binding and allostery in proteins.

Daniel A. Keedy
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Publications


Research Interests

Keywords: structural biology, X-ray crystallography, allostery, bioinformatics, protein design

The Keedy Lab develops experimental and computational methods to control proteins by biasing toward specific conformations that underlie functions such as allostery, ligand binding, and catalysis. Our work reveals new opportunities to modulate the activities of therapeutic targets such as tyrosine phosphatases with small molecules and protein engineering, and also offers insights into more general evolutionary processes that led to functional diversity in the human genome.
Khayat group studies the structure and function of proteins encoded for and utilized by pathogens to infect and replicate. We use a combination of X-ray crystallography, cryo-electron microscopy, biophysics, biochemistry, and cellular biology to complete these studies.

Research Interests

Keywords: cryo-electron microscopy, X-ray crystallography, biophysics, biochemistry, cellular biology

We seek to understand the structural and chemical mechanism by which pathogens hijack the cellular machinery of their host for infection and replication. We use a combination of techniques to understand this mechanism at the atomic resolution to relate how chemistry drives biology, and a number of techniques to understand how biology feeds back into chemistry for new pathways to be exploited by the pathogen for infection and replication. We are also interested in developing computational methods to further combine X-ray crystallography with cryo-electron microscopy.
The Kurtzman group focuses on the development of methodologies to characterize the structure and thermodynamics of water on the surface of proteins and the exploitation of solvation properties for the discovery and design of new drugs.

**Publications**

Wickstrom, L. *et al.* Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. *J. Mol. Recognit.* (Accepted Journal of Molecular Recognition)


*Formerly published as T. Young

**Research Interests**

**Keywords:** Solvation Thermodynamics, Statistical Mechanics, Computer Aided Drug Design

Research in the Kurtzman lab focuses on the development of computational tools that can aid in the discovery and rational design of new drugs. His approach applies statistical mechanical theory and computer simulations to better understand the physical principles that govern the molecular recognition between proteins and small molecule ligands (drugs). A particular emphasis is placed on the role that water plays in the molecular recognition process. A principal goal of this research is to help design and discover drugs that bind with high affinity and selectivity to given protein targets.
The Lazaridis lab works in the area of theoretical and computational Biophysics. In the past few years we have worked on the interaction of proteins with biological membranes. We are especially interested in the process of pore formation by antimicrobial peptides and other toxins.

1998-  City College
1992-1998  Postdoc, Harvard University
1987-1992  PhD, University of Delaware

Publications


Research Interests

My research is in the area of Theoretical and Computational Biophysical Chemistry, which aims to understand how biological systems work in terms of the fundamental laws of Physics and Chemistry. Biomolecules, such as proteins and nucleic acids, have well defined conformations which often change in the course of their function. Our goal is to understand the forces that operate within and between biomolecules and develop quantitative mathematical models for their energy as a function of conformation. Such models are useful in many ways, such as predicting the three-dimensional structure from sequence, characterizing conformational changes involved in biological function, or predicting the binding affinity between two biomolecules.
Dr. Sharon Loverde is an Associate Professor of Chemistry at College of Staten Island. Her research group is interested in the area of soft and biological materials.

Publications


Research Interests

Keywords:
The Loverde laboratory utilizes all-atomistic and coarse-grained molecular dynamics simulations to investigate properties of soft and biological materials. We are also interested in characterizing the stability of macromolecular assemblies composed by proteins and/or nucleic acids.
Prabodhika Mallikaratchy

Prabodhika Mallikaratchy develops nucleic acid aptamers against cellular targets to probe cell-cell interactions, receptor-ligands interactions. Her research is highly interdisciplinary, which incorporate organic chemistry, combinatorial screening, structural biology, immunology and biochemistry.

Associate Professor
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2019- current  Associate Professor
2012-2019  Assistant Professor
2008-2012  Research fellow, Memorial Sloan Kettering cancer center
2003-2008  PhD, University of Florida

Selected Publications


For the current list of publications:

Research Interests

Keywords: Nucleic Acid Aptamers (NAAs), Ligand-Guided Selection (LIGS), Nucleic Acid Nanotechnology

Long-term goal of this laboratory is to develop oligonucleotide aptamer based synthetic scaffolds for biological and biomedical applications. Therefore, our research program is aimed at generating new aptamers against biologically important cellular targets, and molecular engineering of multifunctional aptamer structures suitable for drug delivery, imaging and designer immunotherapeutic molecules.
Dr. Louis Massa

Hiroshi Matsui
Professor
Hunter College
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New York, NY 10065
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http://www.hunter.cuny.edu/chemistry/faculty/Lou/Lou

Postdoc: Brookhaven National Laboratory
PhD: Theoretical Molecular Physics, Georgetown University

Publications


Research Interests

Keywords: differential equations, density matrices, density functional theory, Xray crystallography, kernel energy method, information theory,

Applications of Quantum Mechanics to the electronic structure of atoms, molecules, and solids.
Dr. Poget is interested in membrane protein structure and function, with a particular emphasis on the interactions between ion channel domains and animal peptide toxins.

Sébastien Poget
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www.csi.cuny.edu/faculty/POGET_SEBASTIEN.html

2009- current
Assistant Professor, College of Staten Island, CUNY

2003-2009
Postdoc, Albert Einstein College of Medicine, NY

2001-2003
Postdoc, Rockefeller University, NY

1997-2001
PhD, University of Cambridge, UK

Research Interests

Keywords: Solution-state NMR, membrane protein structural biology, ion channels, toxins, electrophysiology, biophysics

The Poget lab is interested in the structural and functional study of membrane proteins through solution-state NMR and other biophysical methods. Our studies focus on better understanding the interactions of animal peptide toxins with their target ion channel domains as tools for an improved understanding of ion channel function and starting point for drug development. To carry out these studies at the cutting edge of structural biology, we are also involved in the development of new and improved methods for membrane protein studies, including development of more powerful membrane mimetics such as bicelles and optimized NMR methods.
Protein-ligand interactions is the unifying theme of my research interests. In particular, the design, synthesis and application of biologically relevant probe molecules to study and elucidate protein-protein and protein-ligand interactions involved in amyloid diseases and cancer.

Adam A. Profit, Ph.D.
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2014- current  Associate Professor of Chemistry
2004-2014  Assistant Professor of Chemistry
2000-2004  Merck Research Laboratories
1997-2000  Postdoc - Albert Einstein College of Medicine
1997  PhD - Stony Brook University

Research Interests

Keywords: Amyloid, protein kinases, peptides, peptoids, enzymology, solid phase synthesis

The abnormal formation of protein aggregates, or amyloid deposits, is the hallmark of Alzheimer’s disease as well as type 2 diabetes. My laboratory is investigating the molecular interactions that occur between key proteins that contribute to the formation of amyloid in these diseases. Through a more detailed understanding of how these proteins self-assembly to form aggregates, we hope to design and develop small molecule and peptide mimetic inhibitors which may serve as potential therapeutic agents.

We are also developing compounds that inhibit the activity of key enzymes (kinases) which can cause tissues to grow out of control and develop into tumors. To accomplish this we are synthesizing molecules that exploit the unique molecular recognition motifs found in these enzymes to more effectively deliver inhibitory species to the active site.

Publications


Publications


Research Interests

Keywords:
Enzyme inhibitors; protein structure and function relationships; cell signaling pathways
Dr. Kevin Ryan

Kevin Ryan, Ph.D.
Associate Professor, Biochemistry Division
Department of Chemistry and Biochemistry
The City College of New York
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2009 - current Associate Professor
2003-2008 Assistant Professor
1996-2003 Postdoc, Columbia University (Chemistry and Biology Depts.)
1996 Ph.D., University of Rochester

Publications

Liu, M. T.; Nagre, N. N.; Ryan, K., Structurally diverse low molecular weight activators of the mammalian pre-mRNA 3' cleavage reaction. *Bioorganic & Medicinal Chemistry* 2014, 22 (2), 834-41;

Li, Y.; Peterlin, Z.; et al., Aldehyde Recognition and Discrimination by Mammalian Odorant Receptors via Functional Group-Specific Hydration Chemistry. *ACS Chemical Biology* 2014;

Lama, L.; Seidl, C. I.; Ryan, K., New insights into the promoterless transcription of DNA coligo templates by RNA polymerase III. *Transcription* 2014, 5 (1);


Research Interests

Keywords: molecular recognition, olfaction, RNA, micro RNA, RNA interference, RNA polymerase III, chemical biology, transcription

In the RNA area, we study the use of chemically synthesized transcription templates as potential information-bearing molecules for producing small therapeutic RNA in human cells. A second RNA area is the biochemistry of RNA processing reactions that occur during the biogenesis of messenger RNA in human cells. In the olfaction area, we use pharmacology, organic synthesis and chemical biology to probe the biochemistry of the sense of smell.
Dr. Ruth E. Stark

Dr. Stark’s biophysics research program focuses on the molecular structure and interactions of protective plant biopolymers, fatty acid-binding proteins that mediate pain and obesity, and melanin pigments associated with human fungal infections.

Research Interests

Keywords: molecular biophysics, biopolymers, bioanalytical chemistry, solid- and solution-state NMR

The Stark Laboratory uses structural biology and biophysical approaches to study plant protective polymers, lipid metabolism, and potentially pathogenic melanized fungal cells. Study of the molecular and mesoscopic architectures underlying the integrity of cuticles in natural and engineered potatoes and tomatoes is undertaken using solid- and solution-state nuclear magnetic resonance (NMR), mass spectrometry, and atomic force microscopy. Ligand recognition and peroxisome proliferator-activated receptor interactions of fatty acid-binding proteins are under investigation by solution-state NMR and fluorescence spectroscopy. The molecular structure and development of melanin pigments within fungal cells are probed using (bio)chemical synthesis and solid-state NMR.

Publications


E. Camacho, C. Chrissian, R.J.B. Cordero, L. Liporagi-Lopes, R.E. Stark, A. Casadevall, N-acetylglucosamine supplementation affects Cryptococcus neoformans cell wall composition and melanin architecture, Microbiology, 2018, 163, 1540-1556.
Maria C. Tamargo is Professor of Chemistry at the City College of New York. Her research is in semiconductor materials and nanostructures design, growth by epitaxial growth techniques, characterization methods, and applications.

Research Interests

Keywords: Molecular Beam Epitaxy, compound semiconductors, II-VI semiconductors, photonic devices, nanomaterials, topological insulators.

Materials growth, properties and applications of semiconductor multi-layered structures grown by molecular beam epitaxy (MBE). Areas of research activity include III-V compounds, strained-layer and short-period superlattices, surface and interface chemistry, visible light emitters, optoelectronic devices, wide bandgap II-VI compounds, II-VI/III-V heteroepitaxy, low dimensional nanostructures, selective area epitaxy, intersubband devices, quantum cascade lasers, VECSELs, topological insulators.

Publications


T. A. Garcia, V. Deligiannakis, C. Forrester, I. Levy and M. C. Tamargo, Bi$_2$Se$_3$ van der Waals Virtual Substrates for II–VI Heterostructures, phys. status solidi b 254, 1700275 (2017).
Dr. Mariana Torrente

Dr. Torrente is interested in the molecular mechanisms underlying neurodegenerative and psychiatric disease.

Publications


Research Interests

**Keywords:**

We seek to understand the role of epigenetic mechanisms and protein folding in the etiology of neurodegenerative and neuropsychiatric disease. The central hypothesis of our research is that posttranslational modification (PTM) of histones and protein misfolding play a key role in linking genetic predisposition to cellular toxicity in neurodegenerative disease. Epigenetics and protein aggregation may reveal alternative mechanisms behind the occurrence of disease, serving as the missing link between genetic and environmental factors.