



Sebastian Doniach

Professor of Applied Physics and of Physics, Emeritus

Bio

BIO

How is the function of biomolecules in living systems related to their atomic structure?

Professor Doniach's research group uses scattering of synchrotron X-rays from electron storage rings at SLAC and at the Argonne National Laboratory to study changes in the conformation of molecules as their solvent environments are changed. The research also involves computer simulations of the dynamics and energetic of the resulting changes.

Recent Advances in the biology of DNA have shown that a very large part of the genome in eukaryotes codes for small RNA molecules that appear to be central to the way the genes (coding for proteins) are put together. Doniach's group is currently studying structural changes that occur when some small functional RNA's turn on and off gene expression (riboswitches) without needing to involve protein transcription factors. Understanding RNA control mechanisms is central to our ability to intervene in biological functions such as generation of biofuels by bacteria or of intervention when cells start to go cancerous.

The Doniach group's bio-simulation work involves new ways to represent changes in molecular structure, in which the entire trajectory for a change of conformation is represented in a large number of CPU's where each time slice of the trajectory is managed by one of the CPU's. In this way, a representation of changes involving thousands of degrees of freedom may be obtained at atomic resolution. This method has recently been applied to look at protein misfolding. Another project involves using a highly simplified normal mode representation to represent large scale conformational changes in molecular motor molecules and DNA polymerase.

The group is also working on ways to improve the methods of computing the statistical mechanics of counter-ion shielding of the very large Coulomb forces endangered by the phosphate backbones of DNA and RNA. Software has been developed that modifies the solving of the Poisson Boltzmann equation to include the effects of finite ion size. Further modifications are being worked in to include effects of ion-ion correlations.

Current Area of Focus:

- Membrane Proteins

ACADEMIC APPOINTMENTS

- Emeritus Faculty, Acad Council, Applied Physics
- Member, Bio-X

- Member, Wu Tsai Neurosciences Institute

ADMINISTRATIVE APPOINTMENTS

- Visiting Fellow, Los Alamos National Laboratory, (1987-1991)
- Professor, of Physics and Applied Physics, Stanford University, (1979- present)
- JSPS Visiting Professor, University of Tokyo, (1978- present)
- Professor Associe; 1975-76, 1978, 1982, University of Paris, France, (1975-1982)
- Director, Stanford Synchrotron Radiation Laboratory, (1973-1978)
- Lecturer, Imperial College, (1967-1969)
- Reader in Physics, Imperial College, (1967-1969)
- Lecturer, Queen Mary College, (1960-1964)
- ICI Fellow, University of Liverpool, (1958-1960)

PROFESSIONAL EDUCATION

- Ph.D., University of Liverpool, England , Physics (1958)
- B.A., Cambridge University, England , Physics (1954)

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

Study of changes in conformation of proteins and RNA using x-ray scattering

Teaching

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biophysics (Phd Program)

Publications

PUBLICATIONS

- **Asymmetry in the peak in Covid-19 daily cases and the pandemic R-parameter.** *medRxiv : the preprint server for health sciences*
Bhatkar, S., Ma, M., Zsolway, M., Tarafder, A., Doniach, S., Bhanot, G.
2023
- **Editorial: Structural and quantitative modeling of synapses.** *Frontiers in synaptic neuroscience*
Jung, J. H., Reist, N. E., Doniach, S.
2023; 15: 1254416
- **The transmission of SARS-CoV-2 is likely comodulated by temperature and by relative humidity.** *PloS one*
Raines, K. S., Doniach, S., Bhanot, G.
2021; 16 (7): e0255212
- **The composition of the human ribosome varies significantly in different normal and malignant tissues**
Panda, A. n., Yadav, A. n., Yeerna, H. n., Singh, A. n., Biehl, M. n., Lux, M. n., Schulz, A. n., Klecha, T. n., Doniach, S. n., Khiabani, H. n., Ganesan, S. n., Tamayo, P. n., Bhanot, et al
AMER ASSOC CANCER RESEARCH.2020
- **Tissue- and development-stage-specific mRNA and heterogeneous CNV signatures of human ribosomal proteins in normal and cancer samples.** *Nucleic acids research*
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2020

- **A stochastic model of active zone material mediated synaptic vesicle docking and priming at resting active zones** *SCIENTIFIC REPORTS*
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- **Metal-insulator transition in NiS₂-xSex and the local impurity self-consistent approximation model** *PHYSICAL REVIEW B*
Matsuura, A. Y., Watanabe, K., Kim, C., Doniach, S., Shen, Z. X., Thio, T., Bennett, J. W.
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- **Phase diagram was out of Sync with record** *PHYSICS TODAY*
Doniach, S.
1996; 49 (9): 117-&
- **Simulation of quantum melting of the vortex lattice and of fractional quantum Hall-like states of the quantum vortex liquid in 2D superconductors** *SOLID STATE COMMUNICATIONS*
Onogi, T., Doniach, S.
1996; 98 (1): 1-5
- **Reflections on the superconductor insulator transition**
Doniach, S.
PERGAMON-ELSEVIER SCIENCE LTD.1995: 1601-1603
- **KONDO INSULATORS - ARE SIMPLE THEORIES GOOD ENOUGH**
DONIACH, S., FU, C., TRUGMAN, S. A.
ELSEVIER SCIENCE BV.1994: 450-453
- **PENSON-KOLB-HUBBARD MODEL - A STUDY OF THE COMPETITION BETWEEN SINGLE-PARTICLE AND PAIR HOPPING IN ONE-DIMENSION** *PHYSICAL REVIEW B*
HUI, A., DONIACH, S.
1993; 48 (4): 2063-2073
- **THE READERS NIH** *SCIENCE*
DONIACH, S.
1992; 258 (5082): 531
- **MAGNETISM IN DOPED KONDO INSULATORS** *PHILOSOPHICAL MAGAZINE B-PHYSICS OF CONDENSED MATTER STATISTICAL MECHANICS ELECTRONIC OPTICAL AND MAGNETIC PROPERTIES*
DONIACH, S., FAZEKAS, P.
1992; 65 (6): 1171-1183
- **FERMI-LIQUID PHASE OF THE T-J MODEL AND THE HALL-COEFFICIENT IN HIGH-TEMPERATURE SUPERCONDUCTORS** *PHYSICAL REVIEW LETTERS*
SADEMELO, C. A., WANG, Z. Q., DONIACH, S.
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- **A NEW APPROACH TO A NONLOCAL DENSITY FUNCTIONAL FOR THE CALCULATION OF ELECTRON CORRELATION ENERGIES**
SOMMERS, C., DONIACH, S., FU, C.
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- **THE NATURE OF THE FLUX LATTICE IN ANTIGRANULOCYTES SUPERCONDUCTING NETWORKS** *ZEITSCHRIFT FUR PHYSIK B-CONDENSED MATTER*
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- CZYCHOLL, G., DONIACH, S.
1985; 47-8 (FEB): 17-19
- **A SYSTEM OF 3 JOSEPHSON-JUNCTIONS** *JOURNAL OF APPLIED PHYSICS*
STRENSKI, P. N., DONIACH, S.
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 - **THERMODYNAMICS OF MONOLAYER FORMATION ON AN IMPURE SUBSTRATE - RANDOM-FIELD ISING-MODEL APPROACH** *PHYSICAL REVIEW B*
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 - **K-EDGE X-RAY ABSORPTION-SPECTRA IN AN OCTAHEDRAL ENVIRONMENT - A THEORETICAL AND EXPERIMENTAL-STUDY OF MO(CO)₆** *PHYSICAL REVIEW A*
KUTZLER, F. W., HODGSON, K. O., DONIACH, S.
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 - **MELTING OF 2-DIMENSIONAL VORTEX LATTICES** *PHYSICAL REVIEW LETTERS*
HUBERMAN, B. A., DONIACH, S.
1979; 43 (13): 950-952
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CAILLE, A., RAPINI, A., ZUCKERMANN, M. J., CROS, A., DONIACH, S.
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 - **ZERO-TEMPERATURE REAL-SPACE RENORMALIZATION-GROUP METHOD FOR A KONDO-LATTICE MODEL HAMILTONIAN** *PHYSICAL REVIEW B*
JULLIEN, R., FIELDS, J. N., DONIACH, S.
1977; 16 (11): 4889-4900
 - **THEORY OF CRITICAL-TEMPERATURE OF SUPERFLUID PHASE-TRANSITIONS IN 2 DIMENSIONS** *PHYSICAL REVIEW LETTERS*
DONIACH, S.
1973; 31 (24): 1450-1453
 - **THEORY OF MAGNETIC FLUCTUATIONS IN ITINERANT FERROMAGNETS** *PHYSICAL REVIEW LETTERS*
MURATA, K. K., DONIACH, S.
1972; 29 (5): 285-&
 - **EXCITONS IN MOTT-HUBBARD INSULATORS** *PHYSICAL REVIEW LETTERS*
DONIACH, S., ROULET, B. J., FISHER, M. E.
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- **Predicting recurrence in clear cell Renal Cell Carcinoma**
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- **Observation of correlated X-ray scattering at atomic resolution.** *Philosophical transactions of the Royal Society of London. Series B, Biological sciences*
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Lipfert, J., Doniach, S., Das, R., Herschlag, D.
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- **The Effect of Magnesium on the Thermodynamics of Nucleic Acid Tertiary Contact Formation**
Watkins, H. M., Mendez, D., Ratner, D., Herschlag, D., Doniach, S.
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- **Secondary Structure Elucidation via X-Ray Cross Correlation Analysis**
Lane, T., Mendez, D., Sung, J., Ratner, D., Watkins, H., Doniach, S.
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- **Dependence of Micelle Size and Shape on Detergent Alkyl Chain Length and Head Group** *PLOS ONE*
Oliver, R. C., Lipfert, J., Fox, D. A., Lo, R. H., Doniach, S., Columbus, L.
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- **'Hidden' states are pervasive in RNA folding: detection and dissection through mutate-and-map experiments** *Joint Annual Meeting of the ASPET/BPS at Experimental Biology (EB)*
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- **Salt dependence of the radius of gyration and flexibility of single-stranded DNA in solution probed by small-angle x-ray scattering** *PHYSICAL REVIEW E*
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- **Electrostatics of Nucleic Acid Folding under Conformational Constraint** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Dissecting electrostatic screening, specific ion binding, and ligand binding in an energetic model for glycine riboswitch folding** *RNA-A PUBLICATION OF THE RNA SOCIETY*
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- **The Ligand-Free State of the TPP Riboswitch: A Partially Folded RNA Structure** *JOURNAL OF MOLECULAR BIOLOGY*
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- **Possibility of measuring intrinsic electronic correlations in graphene using a d-wave contact Josephson junction** *PHYSICAL REVIEW B*
Black-Schaffer, A. M., Doniach, S.
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- **Combining Single-Molecule Optical Trapping and Small-Angle X-Ray Scattering Measurements to Compute the Persistence Length of a Protein ER/K alpha-Helix** *BIOPHYSICAL JOURNAL*
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- **Do conformational biases of simple helical junctions influence RNA folding stability and specificity?** *RNA-A PUBLICATION OF THE RNA SOCIETY*
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- **Josephson current in graphene: Role of unconventional pairing symmetries** *PHYSICAL REVIEW B*
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- **Mixing and Matching Detergents for Membrane Protein NMR Structure Determination** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Scaling Behavior of Single Stranded DNA Measured by Small Angle X-ray Scattering**
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- **Effect of nearest neighbor spin-singlet correlations in conventional graphene SNS Josephson junctions** *PHYSICAL REVIEW B*
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