




Michael Levitt

Robert W. and Vivian K. Cahill Professor of Cancer Research and Professor, by courtesy, of Computer Science

Structural Biology

 NIH Biosketch available Online

 Curriculum Vitae available Online

Bio

BIO

The world-wide COVID-19 corona virus pandemic has hijacked all our academic attention. Please see Presentations.

Is it possible to understand the molecular structure and function of proteins and nucleic acids in enough detail to make accurate predictions about structure and function? We are mounting a two-pronged attack on this problem using both molecular dynamics simulation and molecular modeling. (i) Simulation attempts to reproduce the structural, thermodynamic and dynamic properties of a macromolecule in as accurate a way as possible. Starting with simple but realistic expressions for the interactions between atoms and classical laws of motion, we calculate a trajectory that specifies the position and velocity of every atom as a function of time. The time-step between calculated structures is small at 10-15 seconds, and we need to reduce hundreds of thousands of sets of atomic coordinates into a simple coherent description. We have simulated with reasonable fidelity the measurable static and dynamic properties of the several different proteins surrounded by thousands of water molecules. Simulation at different temperatures has allowed exploration of the pathways of protein denaturation of entire proteins and small fragments of protein secondary structure (alpha-helices and beta-hairpins). Companion studies of DNA double-helix segments in solution preserve the classical double helix while still showing a wide repertoire of interesting motions. (ii) Molecular modeling attempts to build a model of a macromolecule using known three-dimensional structures and energy minimization as complementary guidelines. Specific examples of this work include the automatic modeling of antibody variable domains, the general modeling of homologous proteins and studies of DNA base-pair mismatches. Questions we are trying to answer include: How can a protein be stabilized by a single amino acid change? How does the sequence of DNA cause local variations of double-helix conformation and stability? Extensive use is made of sophisticated programming, sequence and structural data bases, and computer graphics.

ACADEMIC APPOINTMENTS

- Professor, Structural Biology
- Member, Bio-X
- Member, Wu Tsai Neurosciences Institute

ADMINISTRATIVE APPOINTMENTS

- Chair, Department of Structural Biology, (1993-2004)
- Associate Chair, Department of Structural Biology, (2005-2010)

HONORS AND AWARDS

- Nobel Prize in Chemistry, Nobel Foundation (2013)
- Member, American Academy of Arts & Sciences (2010)
- Blaise Pascal Professor of Research, Fondation de l'Ecole Normale Supérieure, Paris, France (2003-2004)

- Member, Editorial Board Proc. Natl. Acad. Sci. USA (2002)
- Member, The US National Academy of Science (2002)
- Fellow, The Royal Society (2001)
- Co-director of Program in Mathematics and Molecular Biology, Mathematics and Molecular Biology (1997-2002)
- Anniversary Prize, Federation of European Biochemical Societies (1986)
- Member, European Molecular Biology Organization. (1981)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Member, National Academy of Sciences (2013 - present)

PROFESSIONAL EDUCATION

- PhD, Gonville and Caius College, Cambridge, Structural Biology (1971)

LINKS

- Levitt Site: <http://csb.stanford.edu/levitt/>

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

I pioneered of computational biology setting up the conceptual and theoretical framework for a field that I am still actively involved in at all levels. More specifically, I still write and maintain computer programs of all types including large simulation packages and molecular graphics interfaces. I have also developed a high-level of expertise in Perl scripting, as well as in the advanced use of the Office Suite of programs (Word, Excel and PowerPoint), which is more important and rare than it may seem. My research focuses on three different but inter-related areas of research. First, we are interested in predicting the folding of a polypeptide chain into a protein with a unique native-structure with particular emphasis on how the hydrophobic forces affect the pathway. We expect hydrophobic interactions to energetically favor structure that are more native-like. In this way, the same stabilizing interactions that exist in the final folded state the search tractable. Second we are interested in predicting protein structure from sequence without regard for the process of folding. Such prediction relies on the well-established paradigms that similar protein sequences imply similar three-dimensional structures. We have focused on the hardest problem in homology modeling: the refinement of a near-native structure to make it more precisely like the actual native structure of protein. We have also focused on how the general similarity of all protein sequences resulting from their evolution from common ancestor sequence affects the nature of the protein universe. Third, we are focusing on mesoscale modeling of large macromolecular complexes such as RNA polymerase and the mammalian chaperonin. In this work, done in close collaboration with experimentalists, we use new morphing strategies combined with normal mode analysis in torsion angle space to overcome problems caused by the size and complexity of these critical, biomedically important systems. All this work depends on the way a molecular structure is represented in terms of the force-field that allows calculation of the potential energy of the system. We employ a very wide variety of such energy functions that extend from knowledge-based statistical potentials for a single interaction center per residue to quantum-mechanical force-fields that include inductive effects as well as polarization.

Teaching

STANFORD ADVISEES

Postdoctoral Faculty Sponsor

Joao Pedro Garcia Lopes Maia Rodrigues

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biomedical Informatics (Phd Program)
- Biophysics (Phd Program)

- Structural Biology (Phd Program)

Publications

PUBLICATIONS

- **Comparison of pandemic excess mortality in 2020-2021 across different empirical calculations.** *Environmental research*
Levitt, M., Zonta, F., Ioannidis, J. P.
2022: 113754
- **Accurate determination of solvation free energies of neutral organic compounds from first principles.** *Nature communications*
Pereyaslavets, L., Kamath, G., Butin, O., Illarionov, A., Olevanov, M., Kurnikov, I., Sakipov, S., Leontyev, I., Voronina, E., Gannon, T., Nawrocki, G., Darkhovskiy, M., Ivahnenko, et al
1800; 13 (1): 414
- **Probing Interplays between Human XBP1 α Translational Arrest Peptide and 80S Ribosome.** *Journal of chemical theory and computation*
Di Palma, F., Decherchi, S., Pardo-Avila, F., Succi, S., Levitt, M., von Heijne, G., Cavalli, A.
2021
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *bioRxiv : the preprint server for biology*
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2020
- **Interface: Open-Source Library for Protein Interface Analysis**
Rodrigues, J., Levitt, M.
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- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling** *bioRxiv*
Rodrigues, J. P., Barrera-Vilarmau, S., Teixeira, J. M., Seckel, E., Kastritis, P., Levitt, M.
2020
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *PLoS computational biology*
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- **Solving the structure of Lgl2, a difficult blind test of unsupervised structure determination.** *Proceedings of the National Academy of Sciences of the United States of America*
Ufimtsev, I. S., Almagor, L., Weis, W. I., Levitt, M.
2019
- **Unsupervised determination of protein crystal structures.** *Proceedings of the National Academy of Sciences of the United States of America*
Ufimtsev, I. S., Levitt, M.
2019
- **Automatic Inference of Sequence from Low-Resolution Crystallographic Data.** *Structure (London, England : 1993)*
Ben-Aharon, Z., Levitt, M., Kalisman, N.
2018
- **On the importance of accounting for nuclear quantum effects in ab initio calibrated force fields in biological simulations.** *Proceedings of the National Academy of Sciences of the United States of America*
Pereyaslavets, L., Kurnikov, I., Kamath, G., Butin, O., Illarionov, A., Leontyev, I., Olevanov, M., Levitt, M., Kornberg, R. D., Fain, B.
2018
- **Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial alpha-helical membrane anchors.** *Proceedings of the National Academy of Sciences of the United States of America*
Pataki, C. I., Rodrigues, J., Zhang, L., Qian, J., Efron, B., Hastie, T., Elias, J. E., Levitt, M., Kopito, R. R.
2018
- **Unique function words characterize genomic proteins.** *Proceedings of the National Academy of Sciences of the United States of America*
Scaiewicz, A., Levitt, M.

2018; 115 (26): 6703–8

- **The solution structure of monomeric CCL5 in complex with a doubly sulfated N-terminal segment of CCR5** *FEBS JOURNAL*
Abayev, M., Rodrigues, J. M., Srivastava, G., Arshava, B., Jaremko, L., Jaremko, M., Naider, F., Levitt, M., Anglister, J.
2018; 285 (11): 1988–2003
- **An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12.** *Scientific reports*
Keasar, C. n., McGuffin, L. J., Wallner, B. n., Chopra, G. n., Adhikari, B. n., Bhattacharya, D. n., Blake, L. n., Bortot, L. O., Cao, R. n., Dhanasekaran, B. K., Dimas, I. n., Faccioli, R. A., Faraggi, et al
2018; 8 (1): 9939
- **Emerging β -Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures.** *Journal of the American Chemical Society*
Kang, H., Vázquez, F. X., Zhang, L., Das, P., Toledo-Sherman, L., Luan, B., Levitt, M., Zhou, R.
2017; 139 (26): 8820-8827
- **Future of fundamental discovery in US biomedical research.** *Proceedings of the National Academy of Sciences of the United States of America*
Levitt, M., Levitt, J. M.
2017
- **Sequential allosteric mechanism of ATP hydrolysis by the CCT/TRiC chaperone is revealed through Arrhenius analysis** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Gruber, R., Levitt, M., Horovitz, A.
2017; 114 (20): 5189-5194
- **The language of the protein universe** *CURRENT OPINION IN GENETICS & DEVELOPMENT*
Scaiewicz, A., Levitt, M.
2015; 35: 50-56
- **Birth and Future of Multiscale Modeling for Macromolecular Systems (Nobel Lecture)** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Levitt, M.
2014; 53 (38): 10006-10018
- **WeFold: A coemption for protein structure prediction** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Khoury, G. A., Liwo, A., Khatib, F., Zhou, H., Chopra, G., Bacardit, J., Bortot, L. O., Faccioli, R. A., Deng, X., He, Y., Krupa, P., Li, J., Mozolewska, et al
2014; 82 (9): 1850-1868
- **Deformable elastic network refinement for low-resolution macromolecular crystallography.** *Acta crystallographica. Section D, Biological crystallography*
Schröder, G. F., Levitt, M., Brunger, A. T.
2014; 70: 2241-2255
- **Deformable elastic network refinement for low-resolution macromolecular crystallography** *ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY*
Schroeder, G. F., Levitt, M., Brunger, A. T.
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- **Redundancy-weighting for better inference of protein structural features.** *Bioinformatics*
Yanover, C., Vanetik, N., Levitt, M., Kolodny, R., Keasar, C.
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- **Millisecond dynamics of RNA polymerase II translocation at atomic resolution** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Silva, D., Weiss, D. R., Avila, F. P., Da, L., Levitt, M., Wang, D., Huang, X.
2014; 111 (21): 7665-7670
- **Training-free atomistic prediction of nucleosome occupancy** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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 - **The Crystal Structures of the Eukaryotic Chaperonin CCT Reveal Its Functional Partitioning** *STRUCTURE*
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Kolodny, R., Pereyaslavets, L., Samson, A. O., Levitt, M.
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 - **Evolutionarily consistent families in SCOP: sequence, structure and function** *BMC STRUCTURAL BIOLOGY*
Pethica, R. B., Levitt, M., Gough, J.
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 - **KoBaMIN: a knowledge-based minimization web server for protein structure refinement** *NUCLEIC ACIDS RESEARCH*
Rodrigues, J. P., Levitt, M., Chopra, G.
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 - **Multiscale natural moves refine macromolecules using single-particle electron microscopy projection images** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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2012; 109 (25): 9845-9850
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 - **Comparative modeling and protein-like features of hydrophobic-polar models on a two-dimensional lattice** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
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 - **EVALUATING MIXTURE MODELS FOR BUILDING RNA KNOWLEDGE-BASED POTENTIALS** *JOURNAL OF BIOINFORMATICS AND COMPUTATIONAL BIOLOGY*
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- **Application of DEN refinement and automated model building to a difficult case of molecular-replacement phasing: the structure of a putative succinyl-diaminopimelate desuccinylase from *Corynebacterium glutamicum*** *ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY*
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- **Symmetry-free cryo-EM structures of the chaperonin TRiC along its ATPase-driven conformational cycle** *EMBO JOURNAL*
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- **Optimized Torsion-Angle Normal Modes Reproduce Conformational Changes More Accurately Than Cartesian Modes** *BIOPHYSICAL JOURNAL*
Bray, J. K., Weiss, D. R., Levitt, M.
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- **Remarkable patterns of surface water ordering around polarized buckminsterfullerene** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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- **Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation** *RNA-A PUBLICATION OF THE RNA SOCIETY*
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- **Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure** *STRUCTURE*
Zhang, J., Ma, B., DiMaio, F., Douglas, N. R., Joachimiak, L. A., Baker, D., Frydman, J., Levitt, M., Chiu, W.
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- **Normal Modes of Prion Proteins: From Native to Infectious Particle** *BIOCHEMISTRY*
Samson, A. O., Levitt, M.
2011; 50 (12): 2243-2248
- **Clustering to identify RNA conformations constrained by secondary structure** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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Levitt, J. M., Thelwall, M., Levitt, M.
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Huang, X., Wang, D., Weiss, D. R., Bushnell, D. A., Kornberg, R. D., Levitt, M.
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- **Consistent refinement of submitted models at CASP using a knowledge-based potential** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
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- Minary, P., Levitt, M.
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- **MOTIF-EM: an automated computational tool for identifying conserved regions in CryoEM structures** *BIOINFORMATICS*
Saha, M., Levitt, M., Chiu, W.
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 - **Super-resolution biomolecular crystallography with low-resolution data** *NATURE*
Schroeder, G. F., Levitt, M., Brunger, A. T.
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 - **Mechanism of folding chamber closure in a group II chaperonin** *NATURE*
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 - **Nature of the protein universe** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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 - **Structural Basis of Transcription: Backtracked RNA Polymerase II at 3.4 Angstrom Resolution** *SCIENCE*
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 - **Can Morphing Methods Predict Intermediate Structures?** *JOURNAL OF MOLECULAR BIOLOGY*
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 - **Protein segment finder: an online search engine for segment motifs in the PDB** *NUCLEIC ACIDS RESEARCH*
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Samson, A. O., Levitt, M.
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 - **How hydrophobic Buckminsterfullerene affects surrounding water structure** *JOURNAL OF PHYSICAL CHEMISTRY B*
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Kolodny, R., Koehl, P., Levitt, M.
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PRESENTATIONS

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