Stanford

Michael Levitt

Robert W. and Vivian K. Cahill Professor of Cancer Research

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 Superieure, 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

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biomedical Data Science (Phd Program)
- Biophysics (Phd Program)
- Structural Biology (Phd Program)

Publications

PUBLICATIONS

- **Toward actionable interventions in human aging (12th ARDD meeting, 2025).** *Aging*
  Dekan, A., Lore, S., Yoon, Y. E., Sjöholm, A., Tyshkovskiy, A., Terskikh, A., Cuervo, A. M., Georgievskaya, A., Heinz, A., Seluanov, A., Adams, A., Tsai, A. P., Murray, et al
  2026; 18 (1): 282-302

- **Structure-aware graph learning predicts RNA editability across tissues and species.** *Research square*
  Rosenwasser, Z., Levitt, M., Levanon, E., Oren, G.
  2026

- **Quasi-continuous cotranslational compaction and folding of a multidomain protein.** *bioRxiv : the preprint server for biology*
  Mitsikosta, S., Westerfield, J. M., Pardo-Avila, F., Levitt, M., von Heijne, G., Metola, A.
  2026

- **Reclassification and Weighting of Multiple Causes of Death: US Death Certificates 2003-2023.** *medRxiv : the preprint server for health sciences*
  Levitt, M., Marten, B., Oren, G., Ioannidis, J. P.
  2026

- **ADAR-GPT: A continually fine-tuned language model for predicting A-to-I RNA editing sites.** *Proceedings of the National Academy of Sciences of the United States of America*
  Rosenwasser, Z., Cohen-Fultheim, R., Levitt, M., Levanon, E. Y., Oren, G.
  2026; 123 (2): e2529073123

- **The need to implement FAIR principles in biomolecular simulations.** *Nature methods*
  Amaro, R. E., Åqvist, J., Bahar, I., Battistini, F., Bellaiche, A., Beltran, D., Biggin, P. C., Bonomi, M., Bowman, G. R., Bryce, R. A., Bussi, G., Carloni, P., Case, et al
  2025

- **Single-residue effects on the behavior of a nascent polypeptide chain inside the ribosome exit tunnel.** *bioRxiv : the preprint server for biology*
  Pardo-Avila, F., Kudva, R., Levitt, M., von Heijne, G.
  2024

- **Panel stacking is a threat to consensus statement validity.** *Journal of clinical epidemiology*
  Kepp, K. P., Aavitsland, P., Ballin, M., Balloux, F., Baral, S., Bardosh, K., Bauchner, H., Bendavid, E., Bhopal, R., Blumstein, D. T., Boffetta, P., Bourgeois, F., Brufsky, et al
  2024: 111428

- **The Determination of Free Energy of Hydration of Water Ions from First Principles.** *Journal of chemical theory and computation*
  Butin, O., Pereyaslavets, L., Kamath, G., Illarionov, A., Sakipov, S., Kurnikov, I. V., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskyi, et al
  2024

- **Neural Network Corrections to Intermolecular Interaction Terms of a Molecular Force Field Capture Nuclear Quantum Effects in Calculations of Liquid Thermodynamic Properties.** *Journal of chemical theory and computation*
  Kurnikov, I. V., Pereyaslavets, L., Kamath, G., Sakipov, S. N., Voronina, E., Butin, O., Illarionov, A., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Ivahnenko, I., Chen, et al
  2024

- **Combining Force Fields and Neural Networks for an Accurate Representation of Bonded Interactions.** *The journal of physical chemistry. A*
  Kamath, G., Illarionov, A., Sakipov, S., Pereyaslavets, L., Kurnikov, I. V., Butin, O., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskyi, et al
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- **Variability in excess deaths across countries with different vulnerability during 2020-2023.** *Proceedings of the National Academy of Sciences of the United States of America*
  Ioannidis, J. P., Zonta, F., Levitt, M.

2023; 120 (49): e2309557120

- **Combining Force Fields and Neural Networks for an Accurate Representation of Chemically Diverse Molecular Interactions.** *Journal of the American Chemical Society*
  Illarionov, A., Sakipov, S., Pereyaslavets, L., Kurnikov, I. V., Kamath, G., Butin, O., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskyi, et al
  2023
- **Variability in excess deaths across countries with different vulnerability during 2020-2023.** *medRxiv : the preprint server for health sciences*
  Ioannidis, J. P., Zonta, F., Levitt, M.
  2023
- **What Really Happened During the Massive SARS-CoV-2 Omicron Wave in China?** *JAMA internal medicine*
  Ioannidis, J. P., Zonta, F., Levitt, M.
  2023
- **Flaws and uncertainties in pandemic global excess death calculations.** *European journal of clinical investigation*
  Ioannidis, J. P., Zonta, F., Levitt, M.
  2023: e14008
- **Excess death estimates from multiverse analysis in 2009-2021.** *European journal of epidemiology*
  Levitt, M., Zonta, F., Ioannidis, J. P.
  2023
- **AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor.** *Chemical science*
  Ren, F., Ding, X., Zheng, M., Korzinkin, M., Cai, X., Zhu, W., Mantsyzov, A., Aliper, A., Aladinskiy, V., Cao, Z., Kong, S., Long, X., Man Liu, et al
  2023; 14 (6): 1443-1452
- **Estimates of COVID-19 deaths in Mainland China after abandoning zero COVID policy.** *European journal of clinical investigation*
  Ioannidis, J. P., Zonta, F., Levitt, M.
  2023: e13956
- **Estimates of COVID-19 deaths in Mainland China after abandoning zero COVID policy.** *medRxiv : the preprint server for health sciences*
  Ioannidis, J. P., Zonta, F., Levitt, M.
  2023
- **AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor** *CHEMICAL SCIENCE*
  Ren, F., Ding, X., Zheng, M., Korzinkin, M., Cai, X., Zhu, W., Mantsyzov, A., Aliper, A., Aladinskiy, V., Cao, Z., Kong, S., Long, X., Man Liu, et al
  2023
- **Protein-Ligand Binding Free-Energy Calculations with ARROW—A Purely First-Principles Parameterized Polarizable Force Field.** *Journal of chemical theory and computation*
  Nawrocki, G., Leontyev, I., Sakipov, S., Darkhovskiy, M., Kurnikov, I., Pereyaslavets, L., Kamath, G., Voronina, E., Butin, O., Illarionov, A., Olevanov, M., Kostikov, A., Ivahnenko, et al
  2022
- **Virus spread on a scale-free network reproduces the Gompertz growth observed in isolated COVID-19 outbreaks.** *Advances in biological regulation*
  Zonta, F., Levitt, M.
  2022: 100915
- **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
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- **SARS-CoV-2 Omicron variant: viral spread dynamics, disease burden, and vaccine effectiveness.** *Current medicine (Cham, Switzerland)*
  Sun, S., Wu, J., Chen, R., Levitt, M.
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- **Probing Interplays between Human XBP1u 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
- **The Gompertz Growth of COVID-19 Outbreaks is Caused by Super-Spreaders.** *ArXiv*
  Zonta, F., Scaiewicz, A., Levitt, M.
  2021
- **COMPUTER SIMULATIONS IN SERVICE OF BIOLOGY.** *Frontiers for young minds*
  Levitt, M.
  2021; 8
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *bioRxiv : the preprint server for biology*
  Rodrigues, J. P., Barrera-Vilarmau, S., Teixeira, J. M., Seckel, E., Kastritis, P., Levitt, M.
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- **Interfacea: 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*
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- **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.
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- **Unsupervised determination of protein crystal structures.** *Proceedings of the National Academy of Sciences of the United States of America*
  Ufimtsev, I. S., Levitt, M.
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  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.
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- **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.
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- **Unique function words characterize genomic proteins.** *Proceedings of the National Academy of Sciences of the United States of America*
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- **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.
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- **The language of the protein universe** *CURRENT OPINION IN GENETICS & DEVELOPMENT*
  Scaiewicz, A., Levitt, M.
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- **Birth and Future of Multiscale Modeling for Macromolecular Systems (Nobel Lecture)** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
  Levitt, M.
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- **WeFold: A coopetition 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
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- **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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- **Training-free atomistic prediction of nucleosome occupancy** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Minary, P., Levitt, M.
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- **The Crystal Structures of the Eukaryotic Chaperonin CCT Reveal Its Functional Partitioning** *STRUCTURE*
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  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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- **Improving the Accuracy of Macromolecular Structure Refinement at 7 angstrom Resolution** *STRUCTURE*
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