## Sandor Volkan-Kacso

**Associate Professor** 

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#### HIGHER EDUCATION

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Postdoctoral Fellow	California Institute of Technology	2011 - 2017
PhD, Physics	University of Notre Dame, USA	2011
MS, Computational Physics	Babes-Bolyai University, Romania	2003
BS, Physics	Babes-Bolyai University, Romania	2002
RESEARCH AWARDS & LEADERSHIP		
APU University Award	Undergraduate Scholarly Achievement Award	2023
Research Grants	PI: APU President's Scholarship Enhancement Grant	2022 - 2025
	Co-PI: National Science Foundation, XSEDE <sup>1</sup>	2017
Research Advisor	Caltech Summer Undergraduate Fellowship (SURF)	since 2019
Visiting Fellow	Nanyang Tech. University, Inst. for Advanced Studies	2016
Graduate Fellowship	Center for Applied Mathematics, Univ. of Notre Dame	2009
Visiting Research Fellow	Argonne National Laboratory	2006
Student Conference Prize	OTDK, Hungary	2003
Romanian State Scholarship	Babes-Bolyai University, Romania	1999 - 2002
OTHER ACADEMIC ROLES		
Reviewer	J. Chem. Phys.; J. Phys. Chem., Biophys. J.	since 2014
Chair	Faculty Research Council, Azusa Pacific Univ.	since 2024
Co-chair	Caltech Postdoc Committee (Chemistry and Chemical Eng.)	2015 - 2017

#### PEER-REVIEW PUBLICATIONS

- 21. N. Suiter & S. Volkán-Kacsó, "Angle-dependent rotation velocity consistent with ADP release in bacterial F1-ATPase", *Frontiers in Mol. Biosci.* 10, 1184249 (2023) Link to paper
- 20. S. Volkán-Kacsó and R. A. Marcus, "Theoretical interpretation of F1-ATPase rotary mechanism from single molecule and ensemble kinetic data and structural data", Frontiers in Microbiol, 13, 861855 (2022) Link to paper
- 19. L. Q. Le & S. Volkán-Kacsó, "Fast state detection in F1-ATPase rotation enhanced by theory of mixed states and external torque", *New J. Phys.* 23 (11), 113030 (2021) Link to paper
- 18. S. Volkán-Kacsó and R. A. Marcus "Single Molecule Studies of a Biological Motor F1-ATPase: Interplay of Experiment, Analytic Theory and Computation" in "Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile" Springer Series in Materials Science, vol. 284 (2020) Link to paper
- 17. S. Volkán-Kacsó, L. Q. Le, K. C. Zhu, H. Su and R. A. Marcus "Method to extract multiple states in F1-ATPase rotation experiments from jump distributions", *Proc. Natl. Acad. Sci., USA*, 116, 25456 (2019) <u>Link to paper</u>

<sup>&</sup>lt;sup>1</sup> XSEDE: Extreme Science and Engineering Discovery Environment. Project title "Exploring the rotation of the gamma shaft of F1-ATPase in single-molecule experiments", project number MCB170140, award \$65,394.

- **16. S. Volkán-Kacsó** and R. A. Marcus, "Theory of rate constants of substeps in single molecule experiments on F1-ATPase", in "Oxygen Production and Reduction in Artificial and Natural Systems" Eds. J. Barber, A.V. Ruban and P. J. Nixon, Chap. 2 (2019)
- **15. S. Volkán-Kacsó** and R. A. Marcus, "Theory of single molecule experiments of F1-ATPase: predictions, tests and comparison with experiments", Proceedings of the 24th Solvay Conference on Chemistry 'Catalysis in Chemistry and Biology', World Scientific Publishing Co., Singapore, 285-294 (2018)
- **14. S. Volkán-Kacsó** and R. A. Marcus, "What Can Be Learned about the Enzyme ATPase from Single Molecule Studies of Its Subunit F1?" *Qart. Rev. Biophys.*, **50**, e14 (2017)
- **S. Volkán-Kacsó** and R. A. Marcus, "Long binding events in single molecule controlled rotation in F1-ATPase: Theory and experiment", *Proc. Natl. Acad. Sci., USA,* **114**, 7272–7277 (2017)
- 11. S. Volkán-Kacsó and R. A. Marcus, "Free, stalled, and controlled rotation single molecule experiments on F1-ATPase and their relationships", in *Photosynthesis and Bioenergetics* (Eds. J. Barber and A. V. Ruban), World Scientific Publishing Co., Singapore, 35–53 (2017)
- **10. S. Volkán-Kacsó,** "The elastic transfer model of angular rate modulation in F1-ATPase stalling and controlled rotation experiments", *Mod. Phys. Lett. B*, **31**, 1730002 (2017)
- 9. S. Volkán-Kacsó and R. A. Marcus, "Theory of controlled rotation experiments, predictions, tests and comparison with stalling experiments in F1-ATPase", *Proc. Natl. Acad. Sci., USA* 113 (48), 12029–12034 (2016)
- 8. **S. Volkán-Kacsó** and R. A. Marcus, "Theory of rates and equilibrium constants and Bronsted slopes in F<sub>1</sub>-ATPase single molecule imaging experiments", *Proc. Natl. Acad. Sci., USA*, **112** (46), 14230–14235 (2015)
- 7. Jixin Si, S. Volkán-Kacsó, A. Eltom, Y. Morozov, M. P. McDonald, M. Kuno and B. Jankó, "Heterogeneous fluorescence intermittency in single layer reduced graphene oxide", *Nano Lett.*, **15**, 4317 (2015)
- **S. Volkán-Kacsó**, "Two-state theory of binned photon statistics for a large class of waiting time distributions and its application to quantum dot blinking", *J. Chem. Phys.*, **140**, 2241 (2014)
- 5. P. A. Frantsuzov, S. Volkán-Kacsó, and B. Jankó, "Universality of the fluorescence intermittency in nanoscale systems: experiment and theory", *Nano Lett.*, 13, 402 (2013)
- 4. F. Vietmeyer, S. Volkán-Kacsó, P. A. Frantsuzov, M. Kuno and B. Jankó, "Fluorescence Imaging: Understanding fluorescence blinking is the first path to an imaging solution", *Laser Focus World* 47 (2), (2011)
- 3. S. Volkán-Kacsó, P. A. Frantsuzov, and B. Jankó, "Correlations between subsequent blinking events in single quantum dots", *Nano Lett.* **10** (7), 2416–2420 (2010)
- 2. P. A. Frantsuzov, S. Volkán-Kacsó, and B. Jankó, "Model of fluorescence intermittency of single colloidal semiconductor quantum dots using multiple recombination centers", *Phys. Rev. Lett.* **103**, 207402 (2009)
- 1. Z. Néda, S. Volkán-Kacsó, "Flatness of the setting Sun", Am. J. Phys. 71(4), 379-385 (2003).

#### In preparation

"Correlations in single-molecule imaging of Paracoccus Denitrificans F1-ATPase", S Volkan-Kacso, N Suiter, R Matute and RA Marcus

"Relation between structure and single-molecule rate constants in F1-ATPase", O. Katchikian, S Volkan-Kacso, R Matute and RA Marcus

"Michaelis-Menten kinetics from angle-dependent stepping rate constants in single F1-ATPase", S Volkan-Kacso, N. Panossian and RA Marcus

#### CONFERENCE AND SEMINAR TALKS

• S Volkan-Kacso, *invited speaker*, "Correlation between nucleotide binding and release in the ring-shaped F1-ATPase motors", on "2023 workshop on bidirectional catalysis, from molecular machines to enzymes", Paris, Sept. 11-12, 2023

- S Volkan-Kacso, *invited speaker*, "Interconversion of Chemical and Mechanical Energy in a Biological Motor F1-ATPase", Symposium "Celebrating Rudy Marcus' 100<sup>th</sup> Birthday", Caltech, Jul. 21, 2023
- S Volkan-Kacso, *seminar talk*, "A theory-based method for extracting fast states from single-molecule rotation of F1-ATPase", Semmelweiss University, Budapest, Jun. 30, 2023
- S Volkan-Kacso, *speaker*, "Fast States Revealed by Theory of Jumps in F1-ATPase Rotation Experiments", 64<sup>th</sup> Annual Meeting of the Biophysical Society, Feb. 17, 2020
- S Volkan-Kacso, *seminar talk*, "Method to extract fast states from jump distributions in single-molecule experiments on F1-ATPase", UC Berkeley, Nov. 25, 2019
- S Volkan-Kacso, *invited speaker*, "Competing Angular Velocity and Torque Components in F1-ATPase Rotation Trajectories", Gordon Research Conference on Bioenergetics, June 2-7, 2019
- S Volkan-Kacso, *seminar talk*, "Zooming in on the concerted mechano-biology in single-motor enzymes one substep at a time", Concordia University, Montreal, Feb. 26, 2018
- S Volkan-Kacso, seminar talk, "Concerted mechanics of substeps in single motor enzymes", Miami University, Oxford, Ohio, Feb. 2, 2018
- S Volkan-Kacso, *seminar talk*, "Predictive modeling of single-molecule experiment in fluorescence blinking and motor enzymes", University of Southern California, Apr. 21, 2017
- S Volkan-Kacso, invited speaker, "Theory of the angular modulation of ligand binding rates and equilibrium constants in F1-ATPase controlled rotation experiment", 4<sup>th</sup> International Workshop on Solar Energy for Sustainability: Photosynthesis and Bioenergetics, NTU Singapore, March 22, 2016
- S Volkan-Kacso, "Theory of time-resolved single molecule experiments on the biomolecular motor F1-ATPase", seminar talk, Chemistry and Chemical Engineering Seminar, California Institute of Technology, Oct. 21, 2016
- S Volkan-Kacso, *seminar talk*, "Single molecule imaging and manipulation in F1-ATPase: theory and experiment", Huntington Medical Research Institute, Pasadena, Oct. 4, 2016
- S Volkan-Kacso, *seminar talk*, "Theory of single molecule imaging and manipulation in biomolecular motors", Biophysics Seminar, East Carolina University, April 7, 2016
- S Volkan-Kacso, *seminar talk*, "Group transfer theory of single molecule imaging and manipulation in F1-ATPase", Biological Research Centre, Szeged, Hungary, March 29, 2016
- S Volkan-Kacso and R. A. Marcus, *talk*, "Group transfer theory of single molecule imaging experiments in the F<sub>1</sub>-ATPase biomolecular motor", American Physical Society March Meeting, Baltimore, 2016
- S Volkan-Kacso, *seminar talk*, "Theories of single molecule processes: quantum dot blinking and ATPase rotation", Wigner Research Centre for Physics, Budapest, Jul. 17, 2015
- S Volkan-Kacso, *seminar talk*, "Fluctuations in single molecule spectroscopies: from quantum dot blinking to ATPase rotation", Max Plank Institute for Biophysical Chemistry, Göttingen, Apr. 7, 2014
- S Volkan-Kacso and B. Janko, *talk*, "Blinking in nanoscale systems: a universal theoretical framework", American Physical Society March Meeting 2012
- S Volkan-Kacso, P. Frantsuzov and B. Janko, *talk*, "Theoretical explanation of correlations between on- and off-events in quantum dot fluorescence intermittency", American Physical Society March Meeting 2010 (talk)

## OTHER CONFERENCE PRESENTATIONS

- S Volkán-Kacsó "Theory of torques and fast states in single-molecule observation of a rotary motor" in "22nd European Bioenergetics Conference", Innsbruck, Austria (2024)
- S Volkán-Kacsó "Extracting Short-Lived States In Single F-Atpase Molecular Motors" in "Molecular Biophysics of Membranes", Tahoe, CA (2024)
- S Volkán-Kacsó, LQ Le, NM Suiter\* and RA Marcus. "Fast ADP release in F1-ATPase", Biophys. J., 122 (3), 184a-185a, (2023)

- M Anderson\*, B. Sanei\*, N Suiter\*, S Volkán-Kacsó, "Molecular dynamics simulations of F1-ATPase's angular fluctuations and associated restoring force" Biophysical Journal, 122(3), 137a-138a, (2023)
- Sandor Volkan-Kacso, Rudolph A. Marcus., "Theoretical method for extracting a hidden states in single F1-ATPase rotation experiments", Workshop "Single Biomolecules" at Cold Spring Harbor Lab. (2022).
- S Volkán-Kacsó, LQ Le, NM Suiter and RA Marcus. "Fast ADP release in F1-ATPase", Biophys. J., 122 (3), 184a-185a, (2023)
- M Anderson, B. Sanei, N Suiter, S Volkán-Kacsó, "Molecular dynamics simulations of F1-ATPase's angular fluctuations and associated restoring force" Biophysical Journal, 122(3), 137a-138a, (2023)
- M Anderson, S Volkán-Kacsó, "Molecular Dynamics Simulations of F1-ATPase Using GPU Supercomputer", Bul. Am. Phys. Soc. 66, (2021)
- LQ Le, S Volkan-Kacso "Multi-State Theory of Velocities and Torques in Transitions of Single-Molecule F1-ATPase Rotation", Biophys. J., 120 (3), 172a, 65<sup>th</sup> BPS Annual Meeting (2021)
- NM Suiter, JM Bettencourt, S Volkan-Kacso, RA Matute, "Evaluation of P. denitrificans F1-ATPase Rotary Motion using Automated Methods to Detect Hidden States", Biophys. J. 120 (3), 172a, 65<sup>th</sup> BPS Annual Meeting (2021)
- O Khatchikian, S Volkan-Kacso, "Extracting the Hydrolysis Rate Constant from a Single-Molecule Controlled Rotation Experimental Data on a F1-ATPase", Biophys. J. 118 (3), 132a, BPS Annual Meeting (2020)
- S Volkan-Kacso, LQ Le, H Su, R Marcus, "Fast States Revealed by Theory of Jumps in F1-ATPase Rotation Experiments", Biophys. J. 118 (3), 183a, BPS Annual Meeting (2020)
- RA Matute, S Volkan-Kacso, RA Marcus, "Model for Concerted Power Stroke Generation in Single Myosin V and F1-ATPase Imaging Trajectories", Biophys. J. 118 (3), 355a, BPS Annual Meeting (2020)
- S Volkan-Kacso, "Model for Concerted Power Stroke Generation in Single Myosin V and F1-ATPase Imaging Trajectories", Biophys. J., 116 (3), 277a, BPS Annual Meeting (2019)
- S Volkan-Kacso, "A Theory for Rate Constants in Rotation Trajectories of F1-ATPase", BPS Annual Meeting (2018)
- S Volkan-Kacso, "The angular modulation of binding processes in single molecule stalling and controlled rotation experiments on F1-ATPase", 4th International Workshop on Solar Energy for Sustainability, Nanyang Technological University, Singapore, 2016 (poster)
- S Volkan-Kacso, "Universality of blinking in nanoscale systems: two-state theory vs. multiple recombination centers", CCE Division Seminar Day, Caltech, 2013 (poster)
- S Volkan-Kacso, "Flourescence Dynamics of Nanoscale Materials", Center for Applied Mathematics, University of Notre Dame, 2008 (poster)
- S Volkan-Kacso, P. Frantsuzov and B. Janko, "Uncovering the statistics of fluorescence fluctuation in quantum wires and quantum dots", ACS March Meeting, 2008 (poster)
- S Volkan-Kacso, "Excimer formation of pyrene molecules on gold nanoparticles", ACS Spring Meeting 2007 (poster)
- S Volkan-Kacso, "The Physics of the Setting Sun", Students' Scientific Conference, Debrecen, Hungary 2002 (talk)

### RESEARCH ADVISING AND MENTORING

- Research Advisor, Caltech Summer Undergraduate Fellowship (SURF): Oganes Khatchikian (2019), Nathan Suiter (2020 & 2021), Nayree Panossian (2021), Josiah Emerson (2024), Alexandra Szolnoki (2024)
- Research Advisor, Caltech Amgen Fellows Program: Enzo Florendo (2022)
- Advisor, APU Richter Fellows: Matthew Anderson (2022, 2023), Enzo Florendo (2023), Babak Sanei (2023)
- Physics Senior Thesis Advisor: Matthew Anderson (2023), Oganes Khatchikian (2021)
- Research advisor, Caltech, Luan Le-Quang, visiting fellow, Nanyang Technical University, Singapore: high-speed single-molecule data analysis and modeling in F1-ATPase biomolecular motors (2019))

#### TEACHING EXPERIENCE IN HIGHER EDUCATION

### Associate Professor in Physics, Azusa Pacific University, USA

- o Computational Methods in Physics; upper division Physics (1 semester)
- Electricity and Magnetism; upper division Physics (2 semesters)
- Waves and Optics: upper division Physics majors (3 semesters)
- Writing 2 (Scientific Writing); interdisciplinary STEM majors (1 semester)
- o Physics of Scientits and Engineering 2: lecture (2 semesters) and laboratory (4 semesters)
- o Physics for Life Sciences 2: lecture (3 semesters) and laboratory (3 semesters)

### Adjunct Faculty in Electrical Engineering, Sapientia University, Romania

- Analog Circuits: laboratory (2 semesters)
- Electricity and Magnetism: laboratory: (2 semesters)

# • Teaching Assistant in Physics, University of Notre Dame (2003-2006)

- General Physics lab classes (2003-2005): experiments in Mechanics, Electricity and Magnetism, Thermodynamics.
- Advanced Physics courses (2005-2006): Solid State Physics, Quantum Mechanics III (graduate), Manybody Physics

### PROFESSIONAL MEMBERSHIPS

- Member: American Chemical Society, American Physical Society, American Biophysical Society
- Member: US West Coast Club of Hungarian Scientists

## SCIENTIFIC COMPUTER PROGRAMMING

### Atmospheric light refraction -- computer software:

- o SPC Sun Position Calculator (free) http://phys.ubbcluj.ro/~zneda/suncalc/spc/
- Visual simulation software of sunset with atmospheric refraction
- o algorithms in C++ to calculate the light path through the atmosphere using the law of refraction
- o algorithms in Visual C++ to visualize the light path and a Windows App to calculate corrections to the Sun's position given by model parameters (time, location, temperature, etc)

### Molecular dynamics simulation of nanostructures:

- o algorithms for simulated annealing in C++ to construct the initial coordinates for nanocrystal surface
- algorithms in TCL scripting language to evaluate MD simulation results of the above structure. Large simulation trajectory ("dig data") "reduced" to extract essential info before the era of big data

## • Photon counting statistics:

- MATLAB scripts to solve parametrized kinetic equations, effectively parameterized first order ODEs.
  Code optimized for vectorization (MATLAB's fast this way), elementary inverse Laplace transform implemented, solutions found for tensor operations and parallelization
- shell (ba) scripting for parallel jobs (mostly SMP) using Sun Grid Engine (including MD simulations)

# • Visualization of data and concepts:

 MATLAB code, Grace scripting to generate technical figures. ImageJ scripting (Java based) for imaging spatio-temporal data. Tcl scripting to visualize large biomolecules and their simulation data. Vector graphics (CorelDraw, InkScape) for diagrams. MS Power Point animations to support scientific talks. Poster creation with MS Publisher