Sándor Volkán-Kacsó, PhD

Associate Professor

T: 626-815-6000 ext. 6614 | E: skacso@apu.edu

PREVIOUS APPOINTMENTS

Senior Postdoctoral Researcher	California Institute of Technology	2017 – 2018
Postdoctoral Scholar	California Institute of Technology	2011 – 2017
Research Assistant	University of Notre Dame, Department of Physics	2006 – 2011
Teaching Assistant	University of Notre Dame, Department of Physics	2003 – 2006
Adjunct Faculty	Sapientia Technical University, Romania, Department of Electrical Engineering	2002 – 2003

HIGHER EDUCATION

PhD, Physics	University of Notre Dame	2003–2011
MS, Physics	University of Notre Dame	2003–2007
MS, Computational Physics	Babes-Bolyai University, Romania	2002–2003
BS, Physics	Babes-Bolyai University, Romania	1998–2002

PUBLICATIONS

15. **S. Volkán-Kacsó** and R. A. Marcus "A group transfer model of myosin V power stroke and characteristic distance", *in preparation* (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)

13. **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)

12. **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)

11. **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)

10. **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)

10. **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 (2016)

8. **S. Volkán-Kacsó** and R. A. Marcus, "Theory of rates and equilibrium constants and Bronsted slopes in F_1-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)

6. **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

16. "Elastic model for velocity profiles in A- and F-ATPases" L. Le Quang, H. B. Su and S. Volkán-Kacsó

17. "Dynamics of N-vacancy blinking in nanodimonds" S. Volkán-Kacsó, C. Bradac, A. Zvyagin and B. Janko

18. Conformational dynamics simulation of excimer formation experiments on plasmonic nanoparticles", S. Volkán-Kacsó, I. Kosztin and B. Jankó

19. "Elasto-chemical theory of torque and force generation in ring-structured ATPase rotation and pulling experiments" S. Volkán-Kacsó

INVITED CONFERENCE AND SEMINAR TALKS

- "Zooming in on the concerted mechano-biology in single-motor enzymes one substep at a time", Concordia University, Montreal, Feb. 26, 2018
- "Predictive modeling of single-molecule experiment in fluorescence blinking and motor enzymes", University of Southern California, Apr. 21, 2017
- "Theory of the angular modulation of ligand binding rates and equilibrium constants in F1-ATPase controlled rotation experiment", 4th International Workshop on Solar Energy for Sustainability: Photosynthesis and Bioenergetics, NTU Singapore, March 22, 2016
- "Theory of time-resolved single molecule experiments on the biomolecular motor F1-ATPase", Chemistry and Chemical Engineering Seminar, California Institute of Technology, Oct. 21, 2016
- "Single molecule imaging and manipulation in F1-ATPase: theory and experiment", Huntington Medical Research Institute, Pasadena, Oct. 4, 2016
- "Theory of single molecule imaging and manipulation in biomolecular motors", Biophysics Seminar, East Carolina University, April 7, 2016
- "Group transfer theory of single molecule imaging and manipulation in F1-ATPase", Biological Research Centre, Szeged, Hungary, March 29, 2016
- "Theories of single molecule processes: quantum dot blinking and ATPase rotation", Wigner Research Centre for Physics, Budapest, Jul. 17, 2015
- "Fluctuations in single molecule spectroscopies: from quantum dot blinking to ATPase rotation", Max Plank Institute for Biophysical Chemistry, Göttingen, Apr. 7, 2014

OTHER CONFERENCE PRESENTATIONS

- "A Theory for Rate Constants in Rotation Trajectories of F1-ATPase", Biophysical Society Meeting, San Francisco, 2018 (poster)
- "Group transfer theory of single molecule imaging experiments in the F_1-ATPase biomolecular motor", American Physical Society March Meeting, Baltimore, 2016 (talk)

- "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)
- "Universality of blinking in nanoscale systems: two-state theory vs. multiple recombination centers", CCE Division Seminar Day, Caltech, 2013 (poster)
- "Blinking in nanoscale systems: a universal theoretical framework", American Physical Society March Meeting 2012 (talk)
- "Theoretical explanation of correlations between on- and off-events in quantum dot fluorescence intermittency", American Physical Society March Meeting 2010 (talk)
- "Flourescence Dynamics of Nanoscale Materials", Center for Applied Mathematics, University of Notre Dame, 2008 (poster)
- "Uncovering the statistics of fluorescence fluctuation in quantum wires and quantum dots", ACS March Meeting, 2008 (poster)
- "Excimer formation of pyrene molecules on gold nanoparticles", ACS Spring Meeting 2007 (poster)
- "The Physics of the Setting Sun", Students' Scientific Conference, Debrecen, Hungary 2002 (talk)

PROFESSIONAL MEMBERSHIPS AND COMMITTEES

- Reviewer: Journal of Chemical Physics, Journal of Physical Chemistry
- Co-chair: Caltech Chemistry and Chemical Engineering Postdoc Committee
- Member: American Chemical Society, American Physical Society, American Biophysical Society
- Member: US West Coast Club of Hungarian Scientists
- Board member: Caltech Postdoctoral Association, Career Committee

TEACHING EXPERIENCE IN HIGHER EDUCATION

- **Adjunct Faculty in Electrical Engineering, Sapientia University, Romania.**
  - Analog Circuits laboratory: set up and teach laboratory classes, evaluate term papers
  - Electricity and Magnetism laboratory: design, set up, and teach laboratory classes, evaluate term papers
  - High-load, high-responsibility teaching environment in a start-up institution
- **Teaching Assistant of Physics, University of Notre Dame (2003-2006).**
  - General/introductory Physics lab classes (2003-2005): set up and assist with experiments in Mechanics, Electricity and Magnetism, Thermodynamics.
  - Advanced Physics courses (2005-2006): Solid State Physics, Quantum Mechanics III (graduate), Many-body Physics
  - Assisted in preparing and grading exams, problem sets and term papers for Physics curriculum courses at all levels from freshman to advanced graduate.
- **Mentorship in research (2011-)**
  - Jixin Si, U. Notre Dame graduate student: computational modelling techniques for single fluorophore blinking trajectories
  - Luan Le-Quang, Zhihao Liu and Kaicheng Zhu, Nanyang Technological University (Singapore) graduate students: high-speed single-molecule data analysis and modeling in F1-ATPase biomolecular motors

RESEARCH EXPERIENCE AND ACCOMPLISHMENTS

Molecular group transfer theory of F1-ATPase enzyme in relation to single molecule observations. The F_1-ATPase is the water-soluble component of the F-ATPase enzyme, which acts as stepping biomolecular motor. It converts the free energy from the hydrolysis of ATP molecules into directional rotation of its shaft, and works in

reverse compared to the complete F-ATPase. To reveal the molecular mechanism of energy transduction mechanism in the latter, as a postdoctoral fellow at Caltech, I developed an elastic molecular group transfer theory to treat single molecule imaging and "stalling" experiments in the F_1-ATPase. Using an electron or atom transfer theoretical approach the theory couples chemical reactions in the stator and the physics of torsional elasticity in the rotor. In the theory we predicted and compared with experiment the rate and equilibrium constant dependence of steps such as ATP binding and phosphate release as a function of the rotor angle. [*PNAS*, **112**, 14230 (2015)]

Theoretical and statistical treatment F_1-ATPase controlled rotation experiments. Using the elastic group transfer theory, in a recent publication I elucidated the mechanism of the exponential-like change of binding and release rates when probed against the rotor angle at the single-molecule level. Using independent experimental data from biochemical ensemble and single-molecule imaging experiments, the model correctly ***predicts the controlled rotation data on fluorescent ATP without any adjustable parameters***. I took into account the biasing effect of finite experimental time resolution in the single fluorescence trajectories and treated these data by developing computational statistical methods.[*PNAS*, **113** (48), 12029 (2016)]

Angular modulation of binding and release of nucleotides in a full 360 degree range. In extending the theory to the full 360 degree range for binding and release a "turnover" in the log of the binding rate versus rotor angle plot is discussed and interpreted in terms of a change from a transfer-control to a diffusion-control, attributed to a narrowing of the channel through which the nucleotide enters into the subunit. A theory-based method for the extraction of rate constants for hydrolysis and synthesis from controlled rotation data was also provided for angular range where no such data is currently available. [*PNAS*, **114**, 7272 (2017)]

The relation between single-molecule experiments in F_1-ATPase and the physiological function of the whole F-ATPase enzyme, composed of the Fo and F1 units. We demonstrated how our elastic molecular transfer theory is able to provide a consistent interpretation and link between the experimental findings. In particular, the theory provided an interpretation of the 360 degree wide angular profile of nucleotide binding and release rate constants in single-molecule controlled rotation experiments, the physiologically relevant chemo-mechanical coupling scheme, the concerted conformational changes in the F1 stator subunits and the central rotor shaft. [*Qart. Rev. Biophys.*, **50**, e14 (2017)]

Multiple recombination model for quantum dot blinking. As a graduate student and later as long-term collaborator I worked in the B. Jankó group at Notre Dame, and helped develop a multiple recombination center (MRC) model of quantum dot fluorescence. This model explained all key features of the quantum dot fluorescence fluctuation ("blinking"). [*Phys. Rev. Lett.* **103,** 207402 (2009)] The most notable of these features include, (1) the (truncated) inverse power-law distribution of on and off times, (2) strong threshold dependence of slope and truncation time, (3) the 1/f power spectrum of the blinking trajectories.

Correlation between consequent on and off times in quantum dot blinking. The MRC model is the first self-consistent model to explain the memory present in blinking. We showed that it can explain the long correlations between subsequent on and off times [*Nano Lett.* **10** (8), 2761–2765 (2010)]. Semi-quantitative agreement has been found in all known features of the correlation, like (1) decay time, (2) strong on-on correlation, (3) negative on-off correlation and (4) weak and identical on-off and off-on correlations. Presently, *no other theory of blinking* is able to reproduce these correlations.

Two-state theory of binned photon statistics for power law blinking. In this project I formulated, execute and published the research as a single author. Using a special kinetic scheme I developed a theory for an extensive class of stochastic waiting time distribution functions, including power laws. I performed a theory and experiment comparison based on a two-level power law system for the intensity histograms of fluorescence trajectories. The observed two peaks were found to be consistent with a distribution of states around a 'bright' and a 'dark' maximum. The findings demonstrated the capability of photon counting theory to achieve super-resolution in the time domain by the ability to treat timescales 100x faster than the experimental resolution. A picture of multiple intensity states for blinking was found to be consistent with the MRC model. [*J. Chem. Phys.,* **140**, 2241 (2014)]

Application of the MRC model to different classes of fluorophores. I developed a robust method to estimate the power spectral density (PSD) of blinking trajectories from several types of fluorophores, colloidal and self-assembled quantum dots, nanowires, nanorods and dye molecules. A unified nonparametric approach based on a

traditional periodogram estimation the method was successfully demonstrated in complicated trajectories with long-time correlations and multiple timescales. It also provides non-trivial confidence interval estimation of the data. Upon the analysis of seven sets of trajectories from different experimental groups I showed that the MRC model can successfully explain the PSD features of these blinking trajectories [*Nano Lett.* **13**, 402 (2013)]

Theory and statistics of blinking in reduced graphene oxide. In this work I extended the theoretical framework of the MRC model and the statistical method for spectrum estimation for the analysis of blinking 2-dimensional graphene-like structures. The analysis revealed the heterogeneous nature of blinking in graphene oxide. The MRC framework was instrumental in the analysis and interpretation of the phenomenon of heterogeneous intermittency. It revealed the evolution of recombination centers during the dynamical photo-reduction process. This work was performed in collaboration with the Kuno (experiment) and Janko (theory) groups. [*Nano Lett.*, **15**, 4317 (2015)]

Statistical analysis of experimental blinking trajectories. A focus of my research is to deal, understand and analyze the "big data": large numbers of often long photon counting fluorescence trajectories resolved in time (avalanche diode) and/or in space (enhanced CCDs). The typical long-range dependence (power law kinetics) of the fluorescent fluctuation renders statistical inference non-trivial. I implemented a Bayesian parameter estimation and model selection method for the on-off threshold analysis of the experimental trajectories received from several experimental groups. I developed a robust method to accurately estimate the power spectral density of the intensity fluctuation (blinking). I analyzed large sets (over 400) of long (10^6 data points) single particle trajectories.

MD simulation of pyrene coating in plasmonic gold nanocrystals. I performed an all-atom molecular dynamics simulation of multiple pyrene molecules attached to gold nanocrystal surfaces. The effect of dimer formation kinetics and excimer fluorescence is studied. The coupling to the plasmon field is taken into account. The NAMD/VMD software package is used with and non-standard force field parameters were calculated using ab-initio electronic structure methods (Gaussian). Dimer formation rates are being calculated in the presence of plasmonic near field, using Kramers theory. [in preparation]

Atmospheric refraction. As an undergraduate student I independently calculated the optical path of solar light traveling through the atmosphere. The calculations explained the apparent flattening of solar rim and shift in elevation due to atmospheric refraction. [*Am. J. Phys.*, **71(4)**, 379-385 (2003)] I developed in Visual C++ a software application that can calculate the solar position (elevation) from any geographic location with corrections due to atmospheric refraction.

RESEARCH INTERESTS

- Novel phenomena and processes in single nanostructures
  - Plasmon-coupled single-particle fluorescence in metal-semiconductor nanostructures
  - Fluorescence enhancement, carrier, exciton and conformational dynamics; surface effects
  - Microscopic mechanism of fluorescence intermittency in semiconductor quantum dots
  - Semiconductor and graphene nanocrystals in energy storage and photovoltaics
- Physics and chemistry of biomolecular motors
  - Rotary (F-ATPase), linear (myosins, kinesins) and revolving motors (motor-DNA complexes)
  - Theory and simulation and of single molecule imaging and manipulation experiments
  - Theories and statistical methods in single molecule fluorescence and force spectroscopies
- "4-dimensional nanoscope" for microsecond resolution biological and nanostructure imaging
  - Time-resolved super-resolution in single particle imaging via statistical modeling
  - Methods in spatio-temporal single particle spectroscopy trajectories (e.g. tracking)
  - Advanced statistical reconstruction imaging via controlled blinking of quantum dots
- Methods for large-scale atomistic simulations in nanoscale heterostructures and biomolecules

COMPUTER PROGRAMMING EXPERIENCE IN RESEARCH

- **Atmospheric light refraction -- computer software:**
  - SPC - Sun Position Calculator (free) http://phys.ubbcluj.ro/~zneda/suncalc/spc/
  - Visual simulation software of sunset with atmospheric refraction

- algorithms in C++ to calculate the light path through the atmosphere using the law of refraction
- 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:**
  - 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

COMMUNITY INVOVEMENT AND OUTREACH

- **Caltech Postdoctoral Association (CPA):**
  - Member of Career and Social Committees
  - Host and organizer of academic career panel discussion on campus
- **Invited panelist UCLA Career Center Inside Careers in Physics Program**
  - 2017 – "Physics Jumpstart @ UCLA" (Feb. 7)
  - 2017 – "Learn at lunch" (Nov. 16)
- **Outreach in K12 education (Sierra Madre, Los Angeles area):**
  - 2013 – LEGO Mindstorms Robotics lab
  - 2014 – Science education (based on the "California Science" curriculum)
  - 2015 – "Biobots" – Elementary School Innovation Club
  - 2017 – Science Olympiad (team coaching)