Annual Report

Theoretical Physics Institute
(founded 1960)

The following pages summarize the activities and publications of Institute Members, Research Associates, Postdoctoral Fellows, Visitors and Graduate Students
For the period of
July 1st, 2011 - June 30st, 2013

Further information can be obtained from:

The Director
Theoretical Physics Institute
Department of Physics
University of Alberta
Edmonton, Alberta T6G 2J1
Canada
http://www.physics.ualberta.ca/
Fax: (780) 492-2150

July 17, 2013

Contents

1 Director's Foreword

Our Theoretical Physics Institute or TPI is now over 50 years old and has continued to provide a focus for work in theoretical physics at the University of Alberta and other nearby institutions. During the report period we have had 28 Active Members from the Departments of Oncology, Chemistry, Engineering, Mathematical Science and Statistics, and Physics at the University of Alberta, as well as from the University of Calgary and University of Waterloo. We also have had 12 Emeritus Members and 3 Honorary Members. With deep sadness we report the passing of our long term members and colleagues, Dr. Donald Betts (TPI director 1972-1978) and Dr. Yasushi Takahashi.

Five of the members are Fellows of the Royal Society of Canada. We have supported 15 postdoctoral fellows and research associates, as well as 67 graduate students. We have hosted one Hiroomi Umezawa Memorial Distinguished Visitor (Sebastien Balibar), one Faculty of Science Distinguished Visitor (John Zarnecki), 14 seminars, 10 long-term visitors, and near 20 short-term visitors.

Our research interests in the TPI include cell biophysics, condensed matter physics, education, gravity and cosmology, quantum computation, mathematical physics, plasma physics, subatomic physics and field theory, theoretical chemical physics, and theoretical geophysics. In the present period we have published two books and over two hundred fifty research papers on subjects ranging from microtubules to gyratons. We have also presented over eighty invited lectures at other institutions.

We are maintaining active interaction with fellow institutions in Korea (Pacific Center of Theoretical Physics and Kunsan National University) and Japan (Yukawa Institute for Theoretical Physics, Kyoto) and in 2013 initiated signing of the MOU between the Faculty of Science and Charles University (Pargue, Czech Republic).

Thus it has been a very active period for the Theoretical Physics Institute, and the impact of our work has been felt worldwide.

2 TPI membership

2.1 Council of the Institute

The Council includes Ex-officio, Active and Associate members with the Director as Secretary:

Director Dmitri Pogosyan, *Department of Physics*

Ex-officio

- Mauricio Sacchi, *Chair, Department of Physics*
- Bin Han, *Director, Applied Mathematics Institute*
- Jonathan Schaeffer *Dean, Faculty of Science*
- Lorne Babiuk *Vice-President Research*

Honorary members

- D.D. Betts R. Ph.D. (McGill), F.R.S.C.
- W. Israel Ph.D. (Montreal), Ph.D. (Dublin), F.R.S., F.R.S.C.
- H.J. Kreuzer Ph.D., D.Sc. (Germany), F.R.S.C.

Active members

- K. Beach Ph.D. (MIT)
- V. Bouchard, Ph.D. (Oxford)
- S. Bhattacharjee Ph.D. (Indian Institute of Technology, India)
- J. Bowman Ph.D. (Princeton)
- A. Brown Ph.D. (University of Western Ontario)
- A. Czarnecki Ph.D. (University of Alberta)
- C. Doran Ph.D.
- V. P. Frolov Ph.D. (P.N. Lebedev Physical Institute)
- T. J. Gannon Ph.D. (McGill)
- G. Hanna Ph.D. (University of Toronto)
- N. Ivanova Ph.D. (Oxford)
- F. Khanna Ph.D. (Florida State)
- M. Klobukowski Ph.D. (Nicolas Copernicus University)
- M. Legare Ph.D. (Université de Montréal)
- F. Marsiglio Ph.D. (McMaster University)
- M. de Montigny Ph.D. (Université de Montréal)
- S. Morsink Ph. D. (University of Alberta)
- D. Page Ph.D. (Cal. Tech.)
- A. Penin Ph.D. (Moscow Institute for Nuclear Research)
- D. Pogosyan Ph.D. (Tartu University)
- P. N. Roy Ph.D. (Université de Montréal)
- W. Rozmus Ph.D. (Warsaw)
- M. Sacchi Ph.D. (UBC)
- B. Sanders Ph.D. (Imperial College, London)
- R. Sydora Ph.D. (University of Texas)
- J. Tuszynski Ph.D. (Calgary)
- E. Woolgar Ph.D. (University of Toronto)
- A. Zelnikov Ph.D. (Moscow Institute of Physics and Technology)

2.2 Emeritus Members

- W. Brouwer Ph.D. (Alberta)
- N. Kamal Ph.D (Liverpool)
- F.C. Khanna Ph.D. (Florida State)
- H.P. Künzle Ph.D. (King's College London)
- G. Ludwig Ph.D. (Brown University)
- R. Moody Ph.D. (University of Toronto)
- B.V. Paranjape Ph.D. (Liverpool)
- M. Razavy Ph.D. (Louisiana)
- H. Schiff Ph.D. (McGill)
- H.S. Sherif Ph.D. (University of Washington)
- Y. Takahashi D.Sc Nagoya (D.Sc.) FRSC
- W. R. Thorson, Ph.D. (CalTech)

3 TPI HQP

3.1 PostDoctoral Fellows/Research Associates

- Tomas Liko, PDF
- Matthew Rupert, NSERC USRA
- Najeh Rekik, PDF
- Holly Freedman, PDF
- Aditya Raghavan, PDF
- Piyush Jain, PDF
- Toby Zeng, NSERC PDF, MRI PDF
- Gregorie Guillon, PDF
- Lecheng Wang, PDF
- Andrei Shoom, RAssoc
- Emmanuel Bongajum, PDF
- Robert Szafron, PDF
- Claude Warnick, PDF
- Nikolai Zerf, PDF
- Christophe Gay, RA

3.2 Graduate students

- Wubshet Alemie, PhD
- Mohammad AlGendy, MSc
- Abdallah Al Zahrani, PhD
- Amsalu Anagaw, PhD
- Giang Bach, PhD
- Marc Baker, MSc
- Khaled Barakat, PhD
- Christopher Bonar, MSc
- Md Mafijul Bhuiyan, PhD
- Carl Chandler, PhD
- Ke Chen, MSc
- Jinkun Cheng, PhD
- Travis Craddock, PhD
- Matthew Dowling, PhD
- Anna Eckl, visiting grad student
- Megan Engel, MSc
- Robert Ferner, MSc
- Christopher Graves, MSc
- Mark Healey, PhD
- Amr Ibrahim, PhD
- Muhammad Junaid, PhD
- Nelson Knutson, MSc
- Nadia Kreimer, PhD
- Gerry Leenders, MSc
- Hongjiang Li, MSc
- Zhou Li, PhD
- Yi Liang, PhD
- Jose Luis Avendano Nandez, PhD

- Niloofar Nayebi, MSc
- Nasser Kazemi Nojadeh, PhD
- Anas Ahmed Othman, MSc
- Konstantin Pavlovskii, PhD
- Christopher Polachic, PhD
- Burkhard Ritter, PhD
- Ismael Vera Rodriguez, PhD
- Karol Rohraff, MSc
- Geoffrey Ryan, MSc
- Kenneth Stanton, PhD
- Abigail Stevens, MSc
- Denis St-Onge, MSc
- Shima Yaghoobpour Tari, PhD
- Christos Tzounis, PhD
- Tyrone Woods, MSc
- Xing Wu, PhD
- Jin Xu, MSc
- Xiaoming Zhang, MSc
- Rui Zheng, PhD
- Fabian Zschocke, visiting grad student
- Shuai Sun, PhD
- Mohammad Momeni Taheri, PhD
- Melis Gedik, PhD
- Mohammad Salem, PhD
- Ekadashi Pradhan, PhD student
- Stephanie Wong, PhD
- Ryan Zaari, MSc
- Tracey Balehowsky, MSc
- Cody Holder, PhD
- Mirza Galib MSc,
- Farnaz Shakib PhD,
- Franz Martinez, MSc
- Tracey Balehowsky, MSc
- Kevin Bishop, Msc
- Nabil Faruk, Msc
- Matthew Schmidt, MSc, NSERC USRA
- Yalina Tritzant, PhD
- Malcolm Roberts, PhD
- Johmwill Keeting, PhD

4 Research Programs

In this section the major achievements and research plans of TPI members are summarized. The areas of research where theoretical physics approaches and methods found fruition range for Cell Biophysics to, obviously, Condensed matter and Particle Physics and Astrophysics, to mathematical subjects related to Quantum Phenomena and Gravitation, to Quantum Computing, Theoretical Chemistry and problems in Engineering.

4.1 Cell Biophysics

Tuszynski, J

Rational Drug Design for Cancer Chemotherapy

The overarching aim of our research activities is to develop and extend existing computational techniques for the rational design of novel drug entities to treat cancer. While there already exists a number of successful drugs to treat many different types of cancer, such as the highly effective paclitaxel, Vinca alkaloids and epothilones, most of these drugs also unfortunately target healthy cells. This often results in therapeutic concentrations of chemotherapy drugs that are only slightly lower than their toxic concentration. Successful chemotherapeutic drugs must therefore take advantage of the differences in the relative vulnerabilities of some target protein or pathway in cancer cells versus normal cells. This has been the premise for research into cancer treatment for several decades, yet a specific, appropriate target has yet to be discovered. To overcome this barrier, numerous molecular targets will be examined for differences at the atomic scale, a process that ultimately involves the rigorous computational analysis of the protein-drug interaction.

This generally involves molecular dynamic (MD) computations, based on atomic-level information about both proteins and drug molecules. Our main objective is to use inexpensive and fast computational techniques to filter large libraries of compounds that will then be subjected to experimental validation. This molecular database screening, coupled with secondary (2D) and tertiary (3D) protein structure analysis and prediction will support the MD model development by limiting the overall search space required.

Our computational research effort comprises an iterative process involving several different modeling techniques to be carried out in the following stages: 1) selection of competent drug targets; 2) molecular refinement of structurally based or homology models; 3) screening and design of suitable drugs; 4) refined modeling of drug-target interactions; and finally 5) classification of candidate drugs into unique QSAR pharmacophores specific for each target protein. Initially, we will create high-resolution meta-models of the drug binding sites for key cell cycle regulatory proteins. These models can either be derived from literature or predicted by using homology modeling algorithms. This provides us with the precise molecular dimensions of each binding site as well as the biochemical and biophysical properties of the constituent amino acids. Using these binding site models, we employ two distinct approaches to characterize molecules that bind at these locations.

Next, high throughput molecular docking simulations are typically performed between each compound in the database (e.g. Cambridge Structural Database or the MDL Chemicals Directory) and each binding site in a given protein. In the docking procedure, the binding orientation of each compound and its binding affinity for the target protein are calculated. Algorithms, such as AUTODOCK, are able to identify small molecules that can fit into the ligand binding sites on proteins of known structure and have been used successfully to identify novel protein-ligand interactions. The docking procedure reduces the number of compound to hundreds or less. These compounds are further filtered with post-screening methods such as detailed MD calculations. These techniques will allow us to probe new or pre-existing drug-binding sites with novel screening methods such as detailed MD calculations. Promising candidates from these screens can then be used as scaffolds to create novel compounds, which can be fed back into the first approach, enhancing binding affinities, hopefully leading to the development of novel drugs for the targeting of cancer cells. The models and simulations described above will be invaluable for rational drug design and study of protein-protein and protein-drug interactions hopefully resulting in pre-clinical development and ultimately clinical trials.

4.2 Colloids and Complex Fluids

Bhattachargee, S.

My current research areas encompass

- Molecular and Interfacial Interactions
- Electrokinetic and Colloid Transport Phenomena
- Complex Fluids, Emulsions, and Petroleum Fluids
- Microfluidics and Nanofluidics
- Water Treatment Technologies
- Water Quality Management

4.3 Condensed Matter Physics

Beach, K.

I am interested in a broad range of problems in condensed matter and computational physics, with strong electronic correlations serving as the dominant theme. I have expertise in several numerical approaches – including quantum Monte Carlo, exact diagonalization, dynamical mean field theory, and optimized trial wavefunctions – with a focus on systems of strongly interacting fermions and spins.

Much of my research has been in the areas of Kondo physics and quantum magnetism. I am interested in the fate of localized moments (electrons) in a material environment, and I investigate what kinds of ground states can be stabilized with simple model Hamiltonians. Some of my current work centres on the search for spin-liquid and bond-crystal states in frustrated magnets and the characterization of the zero-temperature quantum transitions at their phase boundaries. I also put considerable effort into the improvement of existing numerical methods and the development of new ones. The goal here is to push the envelope of what can be simulated with unbiased methods and to extend our capabilities of quantitative detection and characterization to encompass new aspects that have not traditionally been measured in simulations. The latter includes, for example, topological properties, quantum entanglement, Marshall-Peierls sign structure, emergent degrees of freedom, and strongly out-of-equilibrium quantum dynamics.

Additionally, in the last two or three years, I have encouraged my group to develop new expertise in diverse areas of condensed matter – including quantum nanoscience and biophysics – outside our usual purview. This was driven by a desire to connect with the amazing basic and applied research going on around us and to better align ourselves with (highly targeted) provincial funding opportunities. We now have active collaborations with experimentalists in our own Department and with researchers at the National Institute for Nanotechnology (NINT), which sits adjacent to Physics on the University of Alberta campus.

Marsiglio, F.

We know that electrons in solids can do some very impressive things; exotic magnetic states, superconductivity, various charge ordered states, quantum hall effect, etc. What makes this so? The answer seems to be that electrons establish many-body correlations, based on a competition of sorts, between their tendency to minimize their kinetic energy vs. their potential energy as they strive to lower their overall energy. In the last three decades or so, the sub-field of so-called 'strongly correlated electron systems has emerged as an important area of study, somewhat as a reaction to the description of the exotic states mentioned above based primarily on kinetic energy-driven considerations, which is a loose way of characterizing so-called Fermi Liquid Theory.

In strongly correlated electron systems the idea that the Fermi sea is a starting point is challenged, and researchers turn to the Coulomb interactions in the problem as a more viable starting point. The most common paradigms are the Hubbard and the Holstein models for electron-electron and electron-phonon interactions, respectively. In one aspect of our research program we investigate to what extent Fermi Liquid-based descriptions stand up to accurate solution of these models. For example, an exact numerical solution, in the thermodynamic limit, is now accessible for the so-called "polaron" problem, where a single electron interacts with an array of vibrating ions. While this problem was historically important in semiconductors, it is also relevant to superconductivity and charge density waves, as the polaron (electron dressed with local phonon excitations) is the 'basic building block for these many body states. Ongoing work continues with more complicated models, and an attempt to understand the properties of a macroscopic number of polarons.

Another area of our research program questions whether the Coulomb interactions are sufficient to capture the proper correlations that lead to the aforementioned exotic states. For example, the so-called 'Dynamic Hubbard model suggests that Coulomb interactions affect the electron kinetic energy and vice versa, and that they are not simply independent ingredients of the Hamiltonian. Recent progress utilizes Dynamical Mean Field Theory (DMFT) methods.

4.4 General Relativity, Cosmology and Theoretical Astrophysics

Frolov, V.

My research during the past 3 years focused on problems of the black hole physics. The most interesting results were obtained in the following directions:

• Higher dimensional black holes, hidden symmetries and separation of variables. In 2006 we (with my previous PhD student David Kubiznak) discovered that all rotating black holes with spherical topology of the horizon in any number of spacetime dimensions possess a universal generator of a complete set of explicit and hidden symmetries. As a result the equation of motion of particles and light are completely integrable in these spacetimes and the main field equations in these metrics can be solved by the method of separation of variables. During the past year I and my collaborators continued study remarkable properties of the higher dimensional black hole solutions. First important result, obtained in this direction is that similar properties (complete integrability and complete separability) is valid for Dirac equations in a wide class of (weakly) electrically charged rotating black holes. Second result concerns generic geometrical structures in a spacetime of a higher dimensional black hole. Well known examples of dynamical systems that have the property of the complete integrability, possess so called Lax pairs, that is special type of matrices obeying the Lax pair equations. We demonstrated that in the higher dimensional black holes such Lax pairs also exist and we constructed these matrices explicitly in terms of the fundamental generators of explicit and hidden symmetries. It should be emphasized that there exist quite restricted number of known completely integrable dynamical systems. Our result allows one to generate infinite number of new physically interesting examples of such systems.

• Properties of magnetized black holes. There are evidences that magnetic field plays an important role in astrophysical black holes. In particular, it may provide mechanism explaining the energy transfer from the accretion disk to jets. During the past year we (with my PhD Al Zahrani and PDF Shoom) studied charged particle motion in the vicinity of magnetized black holes. We demonstrated that motion of such particles in the equatorial plane (in the accretion disk) is regular (completely integrable), while the motion of such particles out of the equatorial plane is generically chaotic. In particular, we studied the critical escape velocity and demonstrated the near critical motion is chaotic. Using the method of the basin-boundary approach we showed that near critical domain in the space of parameters has fractal structure and determined its fractal dimension. In other words motion of particles that escape from the accretion disc and propagate to the jet domain is similar to the diffusion.

• Relativistic spin-spin interaction We (with my PDF Andrey Shoom) developed modified geometric optics approximation and applied it for study polarized light propagation in the gravitational field of compact massive rotating objects (black holes).

• Classical self-energy and anomaly. The problem of calculation of the self-energy of charged particles has a long history going to classical works of Lorentz, Poincare, Abraham, Fermi and many other famous physicists in the beginning of the past century. In the classical theory the self-energy is divergent in the limit of a point-like charge. Similar (but weaker) divergence is present in the quantum theory. The methods of renormalization were developed in order to extract physical finite value. We applied such covariant methods, well known in the quantum field theory, to study of the self-energy of point-like charges in an external static gravitational field. We demonstrated that this classical problem in D-dimensions can be reduced to the problem of the Euclidean quantum theory in (D-1)-dimensions. The latter one is invariant under a special gauge group. As a result of renormalization this symmetry is broken, so that the classical self-energy contains a contribution of the corresponding anomaly. This result is of general nature. The anomaly does not vanish if D is odd. We calculated this anomaly and applied this approach to study of the interaction of point-like particles with static black holes. Besides possible applications to astrophysical black holes, these results are interesting from theoretical point of view. They demonstrate how well developed techniques of quantum theory can be applied for solving classical problems.

Ivanova, N.

I study interacting binaries, in two main directions: common envelope events and X-ray binaries. In the latter, one stellar companion is a compact object: a neutron star or a black hole. As matter flows from the 'normal' star onto a compact object, the potential energy released is emitted in form of X- and gamma-rays. The tremendous amount of the released energy makes such 'X-ray binaries' stand out even when they are located in very distant galaxies. They thus act as beacons, and their rate of occurrence is among our best clues for the population of massive stars there. The key to understand X-ray binaries in "a field" of a galaxy is in the preceding, unseen interaction - the so-called "common envelope event" (CEE), which is the most important event in the lives of close binary stars. During CEE, binary companions share their outer layers, and as a result they either form a compact binary which could become an X-ray binary, or merge into a single object. In globular clusters – spherical collections of millions of stars in a very compact space – X-ray binaries are formed differently from field ones, as they are formed via collisional interactions. The X-ray binaries in globular clusters are our keys to understand overall dynamics of those spherical collections of stars.

CEEs are believed to be the vital to explain many extremely important and high-energy events in the Observable Universe, such as Type Ia supernovae, X-ray binaries, gamma-ray bursts, merging binary black holes and double neutron stars. While the possibility of CEEs has been first proposed almost 40 years ago, astronomers were only able to hypothesize on their occurrence by observing very close binary stars two gravitationally bound stars that orbit each other and separated by less than a solar radius distance – the formation of which could not be explained by any other theory. However, CEEs never were observed in situ, not to the last because it was not known how CEEs could look like. In my published in Science paper we described the observational features that would accompany a common envelope event. In particularly, the model we developed is based on colling-way and recombination model that explain supernova IIp light curves. This has change d the status of common envelope events from non-observable to observed and will allow to study them directly, for the first time. Understanding of how a common envelope event would manifest itself also allowed us to link them to a class of previously mysterious astrophysical events. A collection of red-colored explosions, just little less energetic than supernovae but still extraordinarily immense, had been observed but had lacked a compelling interpretation. Our model explained a significant fraction of these outbursts. This discovery was highlighted in press (both on-line and printed).

I worked intensively also on common envelope physics – on what happens during the event. There exact hydrodynamics calculations not only are notoriously difficult, they can at the moment only cover a span of time which corresponds to an order of magnitude longer than the dynamical time-scale of the system, whereas the full interaction ofter takes multiple thermal-relaxation timescales; and – perhaps most crucially – they depend on so many initial parameters that the meaningful picture is obscured by all these details, many of which likely insignificant. For a 'top-down' approach, there are in essence only two integrals of motion that we can use as starting point: energy and angular momentum.

The 'energy formalism', proposed 30 years ago in 1984, is, to simplify drastically, simply the parameterization of mechanical energy loss in the form $\alpha \Delta E_{orbital} = E_{envelope}$. On the LHS we have the difference in the orbital energy before and after the even, and the RHS is the binding energy the envelope had had before it was shunned. With the wealth of new observations now available, one can try to calibrate the 'efficiency' parameter – indeed, many observers did – but one runs in a number of unpleasant surprises.

I have shown that two separate modifications are needed to correct the classical energy-balance approach. First, it must be realized that the RHS is extremely ambiguous – there was until now no definition of where a core ends and envelope begins which is based on a physical principle rather than arbitrary. This boundary is what I called in my report as 'what is left from the star'. The arbitrariness of choosing the division allows an uncertainty of two orders of magnitude in the balance – and yes, many publications have abused this choice to tweak their results.

The key to finding this 'bifurcation point' inside the star is to realize the second problem with the energy equation, namely that it does not account for the energy which can be released from the compressed gas in the lower layers of the envelope.

A somewhat culmination of my work on physics of the process is a very large review paper devoted to CEE physics (73 pages not counting supporting material that described a new numerical method).

Together with Craig Heinke, I worked on understanding of the observed ultra-compact X-ray binaries, where the detected X-ray luminosity is by about 2 orders of magnitude exceeds the theoretically expected one. I proposed that this is because a donor is not a remnant of a low-mass white-dwarf, but of a helium core of an intermediate star that retained enough entropy to remain non-degenerate to explain high mass transfer rates.

I resolved the old-standing puzzle about dynamical formation of X-ray binaries in globular clusters and explained why metal-rich clusters form them three times more efficiently than metal-poor clusters. Importance of the explanation and its elegant simplicity warranted its speedy publication in the Astrophysical Journal Letters.

Morsink, S.

Over the last few years my research has focused on an effort to constrain the interior physics of neutron stars through the periodic X-rays observed. If light is emitted from the surface of a rotating star, a periodic signal is observed. If the gravitational field is high, light will be bent around the star, making the spot visible for a larger fraction of the period than for a star described by Newtonian gravity. Hence the gravitational lensing effect makes the light curve less modulated. This modulation depends on the surface gravitational field M/R. The rapid rotation introduces Doppler effects that create asymmetries in the light curve which are proportional to $R\Omega/c$ where the star's angular velocity Ω is easily determined from observations. The main idea is to analyse the observed light curves and detect these two effects which then constrain M and R, assuming the other aspects of the microphysics are well-determined. The Large Observatory for X-ray Timing (LOFT) is a proposed X-ray satellite that is competing to be launched by the European Space Agency's (ESA). LOFT is one of 4 missions (selected through an earlier competition) to be invited to compete, and if successful will be launched around the year 2020. I was invited to join the LOFT "Dense Matter" Science Group, which is working to provide the science case for how LOFT can be used to constrain the properties of the dense matter found in neutron stars. I am collaborating with other members of this group on testing out how well LOFT could help constrain neutron star properties. This is very important, since it is considered to be one of LOFT's major scientific goals. When the ESA evaluates the proposed missions, they will make their decision based on many factors, such as the engineering feasibility as well as how interesting the science is and whether the science goals can be met.

Page, D.

For the reporting period I would like to highlight the following research in the theory of gravity and quantum cosmology

In "Massless Scalar Field Vacuum in de Sitter Spacetime," my graduate student Xing Wu and I looked at the old problem Bruce Allen discovered in 1985, that there exists no de Sitter-invariant Fock vacuum state for a minimally coupled massless scalar field in the de Sitter spacetime. We showed that if one restricts the quantum state to giving expectation values to observables that are invariant under constant shifts in the scalar field, as the action is, then there is a unique de Sitter-invariant vacuum state.

In "Large Randall-Sundrum II Black Holes," my PDFs Shohreh Abdolrahimi and Celine Cattoen and my Ph.D. student Shima Yaghoobpour Tari and I presented a brief form of the numerical solution we found for black holes in the Randall-Sundrum II braneworld model, in which our universe resides on a four-dimensional brane sitting in a bulk five-dimensional spacetime obeying the vacuum Einstein equations with a negative cosmological constant away from the brane. Such a solution had been doubted in several previous papers.

Besides the short Letter on the Randall-Sundrum II black hole solution that we have found, Shohreh Abdolrahimi, Celine Cattoen, Shima Yaghoobpour Tari, and I also wrote up a longer paper, "Numerical Solutions for Large Static Randall-Sundrum II Black Holes," which gives many more of the details about our numerical solution and comparison with the independent but earlier results of Figueras, Lucietti, and Wiseman. Even though our methods were quite different, our numerical results are in close agreement.

In "Statistical Evidence Against Simple Forms of Wavefunction Collapse," I showed that if the initial quantum state of the universe is a multiverse superposition over many different sets of values of the effective coupling 'constants' of physics, and if this quantum state collapses to an eigenstate of the set of coupling 'constants' with a probability purely proportional to the absolute square of the amplitude (with no additional factor for something like life or consciousness), then one should not expect that the coupling 'constants' would be so biophilic as they are observed to be. Therefore, the observed biophilic values (apparent fine tuning) of the coupling 'constants' is statistical evidence against such simple forms of wavefunction collapse.

Recently there has been much discussion as to whether 'old' black holes (which is taken to mean older than what has become known as the 'Page time,' the time at which the von Neumann entropy of the Hawking radiation from a black hole reaches its maximum, after old calculations of mine showing that the peak is very sharp) have firewalls at their surfaces that would destroy infalling observers. Though I suspect that a proper handling of nonlocality in quantum gravity may show that firewalls do not exist, in "Hyper-Entropic Gravitational Fireballs (Grireballs) with Firewalls," I proposed an extension of the firewall idea to what seems to be the logically possible concept of hyper-entropic gravitational hot objects (gravitational fireballs or grireballs for short) that have more entropy than ordinary black holes of the same mass.

In "Exact Quantum Statistical Dynamics of Time Dependent Generalized Oscillators," my former graduate student (and now Professor of Physics at Gunsan National University in Korea) and I used linear invariant operators in a constructive way we find the most general thermal density operator and Wigner function for time-dependent generalized oscillators.

In “Generalized Jarzynski Equality,” I gave a generalization, relating any two quantum states of a system, of the Jarzynski equality that equates the mean of the exponential of the negative of the work (per fixed temperature) done by a changing Hamiltonian on a system, initially in thermal equilibrium at that temperature, to the ratio of the final to the initial equilibrium partition functions of the system at that fixed temperature.

If a black hole starts in a pure quantum state and evaporates completely by a unitary process, the von Neumann entropy of the Hawking radiation initially increases and then decreases back to zero when the black hole has disappeared (with the peak at the so-called ‘Page time’). In “Time Dependence of Hawking Radiation Entropy,” numerical results are given for an approximation to the time dependence of the radiation entropy under an assumption of fast scrambling, for large nonrotating black holes that emit essentially only photons and gravitons. The maximum of the von Neumann entropy then occurs after about 53.81% of the evaporation time, when the black hole has lost about 40.25% of its original Bekenstein-Hawking (BH) entropy and then has a BH entropy that equals the entropy in the radiation, which is about 59.75% of the original BH entropy $4\pi M_0^2$, or about $7.509 M_0^2 \approx 6.268 \times 10^{76} (M_0/M_\odot)^2$, using my 1976 calculations that the photon and graviton emission process into empty space gives about 1.4847 times the BH entropy loss of the black hole.

In “Excluding Black Hole Firewalls with Extreme Cosmic Censorship”, I have given my latest idea for how to avoid the shocking argument of Almheiri, Marolf, Polchinski, and Sully (AMPS) that an “infalling observer burns up at the horizon” of a sufficiently old black hole, so that the horizon becomes what they called a “firewall.” The AMPS argument for black hole firewalls seems to arise from an overcounting of internal black hole states that include states that are singular in the past. I proposed to exclude such singular states by Extreme Cosmic Censorship (the conjectured principle that the universe is entirely nonsingular, except for transient singularities inside black holes). I argued that the remaining set of nonsingular realistic states do not have firewalls but yet preserve information in Hawking radiation from black holes that form from nonsingular initial states.

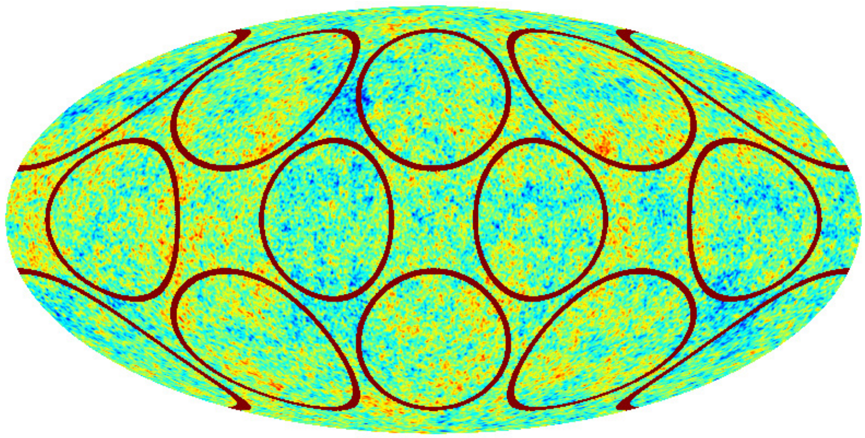
Pogosyan, D

My research interests span the range from the theory of the early Universe and initial perturbations to Cosmic Microwave Background theory and analysis, to the modeling of the observed large-scale structure at low and high redshifts to the statistical study of the galactic turbulence.

Cosmologists are now confident in the overall picture of structure formation in our Universe – the complexity of our Universe came from tiny quantum fluctuations of matter at the early era when the Universe rapidly inflated. Inhomogeneities later grew under the force of gravity into stars, galaxies and, at large scales, the galactic Web, leaving along the way the imprint on the Cosmic Microwave Background (CMB). But fundamental puzzles have also been revealed, among them: What are the ’dark matter’ and ’dark energy’ that successful models have to assume to dominate in the Universe ? How did the filamentary Cosmic Web of galaxies observed in 3D galactic catalogues come into being and is organized ?

Description of the large scale distribution of matter (LSS) and the sky-maps of the polarized CMB radiation involves statistical studies of random fields as the prime methodological approach. It allows, for example, to address such questions as what is the structure of the space of our Universe ? As part of Planck collaboration we placed the limits on the structure of our Universe by studying details of correlation properties in the maps as in the figure below that shows example of CMB temperature map in a small toroidal Universe (circles correspond to physically the same regions of CMB sky observed in different directions. Temperature is expected to be highly correlated between matching pairs of circles)

While the Gaussian limit provides the fundamental starting point in the study of random fields, non-Gaussian features of the CMB and LSS fields are of great interest. Small deviations from gaussianity



in CMB, if detected, could provide a unique window into the details of processes in the early Universe. The gravitational instability that nonlinearly maps the initial Gaussian inhomogeneities in matter density into the LSS induces non-Gaussian features that are essential for quantitative understanding of the filamentary Cosmic Web in-between the galaxy clusters.

We have recently put forward a general formalism for relating measurable geometrical and topological statistics of non-Gaussian random fields to theoretical models. The major advance comes in ability to describe in mildly non-Gaussian regime an extended list of field characteristics, such as densities of extrema or novel statistics related to the field filamentary "skeleton", and in the increased detail the more popular measures, such as topological genus. This opens new ways to contrast non-Gaussian features in observational data (CMB maps, weak lensing convergence maps, 3D galaxy catalogues) to the models. Exploring the possibilities that this formalism entails is one of our objectives. First application to Planck data showed no detectable early non-Gaussianity in the temperature maps. Preliminary estimates show, for example, that topological statistics of lensing convergence maps obtained with proposed Euclid space mission may be competitive in determining "dark energy" parameters. With random fields ubiquitous in physics in areas from turbulence to the landscape of string theories, theoretical advances in their analysis are expected to benefit much wider field than just cosmology.

Building on our expertise in statistical studies of turbulent fluids in interstellar medium, another part of my research is focused on observational signatures of magnetized turbulent astrophysical fluids. In the recent work on synchrotron intensity fluctuations from MHD turbulence we have started to address the main challenge of such theory – the absence of statistical isotropy in the presence of the magnetic field. Using modern, numerically tested, understanding of MHD turbulence we have formulated how locally statistically axisymmetric but globally wandering magnetic field should be statistically described in observer frame and investigated in detail the anisotropic features of different fundamental MHD modes (Alfven, slow and fast). This opens possibilities to use, for the first time with firm understanding, angular dependencies in the observed synchrotron correlation measures to quantify the underlying MHD turbulence.

We advance a novel method of direct studies of the filamentary "skeleton" of the Cosmic Web and its signatures in CMB maps. Our objective is to have full statistical theory of the basic geometrical properties of the skeleton of the Cosmic Web as it evolves. When compared with the properties of the galactic distribution in 3D catalogues, for example, Sloan Digital All Sky Survey, it will allow to constrain the parameters of the still hypothetical "dark energy". We will also gain insight into more intricate properties, i.e. the possible bifurcation patterns and connectivity of the filaments – the issue very interesting for the study of how galaxies assemble into galactic clusters and for modeling the environment in rich cluster conglomerates.

Woolgar, E.

I have focused my recent work on the Ricci flow and its applications in physics. Recent work has concerned the Ricci flow on asymptotically hyperbolic manifolds. With my MSc student Tracey Balehowsky, I was able to compute the behaviour of the asymptotically hyperbolic mass under Ricci flow. Out of this project grew another current project with Eric Bahuaud at Seattle and Rafe Mazzeo at Stanford. We are attempting to show that the Ricci flow of an asymptotically hyperbolic metric with even expansion continues to admit an even expansion throughout the flow. From this, we are able to show that the rate of flow of renormalized volume is governed by the renormalized integral of the scalar curvature. This result may have implications in black hole thermodynamics. I am also interested in the Ricci flow on manifolds with boundary. This is a notoriously difficult problem and little is known. A satisfactory understanding of this flow, however, would have implications for general relativity. In particular, it may provide a way to prove Bartnik's static minimization conjecture, as discussed in the paper with Gulcev and Oliynyk cited above.

Zelnikov, A.

Some of my favorite topics include quantum field theory in curved spacetime, black holes, analogue gravity models, extra dimensions.

• In my recent works with Valeri Frolov we have found a new effect of an anomaly of the self-energy of scalar and electric charges near higher-dimensional black holes. Anomalies are usually considered as a purely quantum phenomenon. But it is not always the case. Quantum field theory methods provided us with the tools to study also a purely classical problem of self-energy of charged particles in higher dimensions, and we found out new features that do not appear in four-dimensional spacetimes.

• I am working on the problem of relation of the area of minimal surfaces in asymptotically AdS spacetimes and the entanglement entropy of quantum fields at the boundary of AdS. This project is related to the hot topic in contemporary theoretical physics: the AdS-CFT correspondence.

• Another topic I am interested in now is the application of methods of quantum field theory in curved spacetime to the calculation of quantum effects (similar to the Unruh effect) in condensed matter systems (like deformed monolayer graphene), where an analogous curved spacetime description emerges naturally.

4.5 Geophysics

Sacchi, M.

My research focus is in the development of numerical techniques to solve inverse problems that arise in seismology. In collaboration with my students, we have been investigating methods to extra extrapolate wavefield in inhomogeneous media. My other research interests include: Bayesian theory applied to inverse problem, estimation theory and higher order statistics.

4.6 Mathematical Physics

Bouchard, V. My research interests focus mainly on the interface between mathematics and physics. More precisely, I am interested in the interconnections between string theory, geometry, topology, number theory, quantum field theory and gauge theory.

Bowman, J. My past work on the analytical and numerical aspects of statistical closures in turbulence has led to the recent development of Spectral Reduction, a reduced statistical description of turbulence. The agreement with full numerical simulations appears to be remarkably good, even in flows containing long-lived coherent structures. Among the practical applications, such a tool can be used to assess the effect of various dissipation mechanisms in large-eddy simulations, as a subgrid model, or even as a substitute for full simulation of high-Reynolds number turbulence.

My other research interests include: implicit dealiasing of linear convolutions, 3D vector graphics, inertial-range scaling laws for two-dimensional fluid, plasma, and geophysical turbulence; nonlinear symmetric stability criteria for constrained non-canonical Hamiltonian dynamics; turbulent transport and the role of anisotropy in plasma and geophysical turbulence; realizable statistical closures; electro-osmotic flow; parcel advection algorithms; exactly conservative integration algorithms; anisotropic multigrid solvers.

de Montigny, M.

My general research program concerns applications of symmetries, Lie algebras and their representations, in field theory. After completing work on contractions of infinite-dimensional Kac-Moody algebras in collaboration with Claudia Daboul (UK) and Jamil Daboul (Israel), I am currently studying contractions of Kac-Moody superalgebras. In collaboration with Faqir Khanna (U of A) and many collaborators, we have worked on a Lorentz-like approach to Galilean covariance based on a (4+1)-dimensional space-time; this allows us to describe non-relativistic systems (for instance, in condensed matter physics, many-body systems) using some well-known techniques of Lorentz-covariant (that is, relativistic) theories.

Legare, M.

A study of properties and characteristics of certain differential equations of the ordinary and partial types, where use is made of different products such as noncommutative and nonassociative products, has been continued. For example, integrable aspects, symmetries, and formulations on superspaces have been considered.

4.7 Plasma Physics

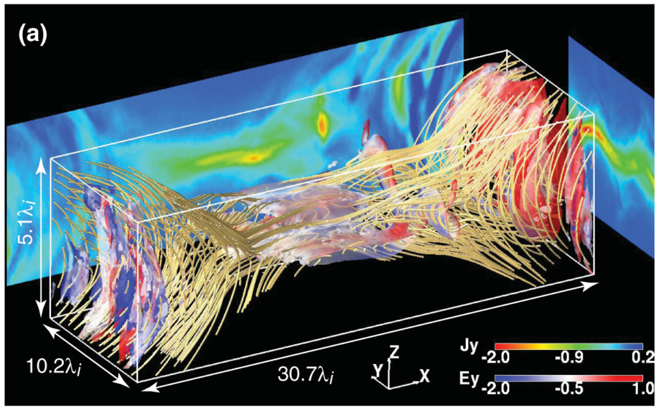
Rozmus, W.

My research has been focused on theoretical and computational plasma physics. Theoretical problems in plasma science are formidable. The goal is to achieve quantitative understanding of nonlinear, many body processes in ionized gases often out of equilibrium. I have contributed over the years to the development of theoretical and numerical methods in plasma theory, with emphasis on nonlinear phenomena, transport and kinetic theory. These theoretical models have been applied in the interpretation of plasma laboratory experiments, with particular attention to laser plasma interaction experiments.

For several decades the field of laser matter interaction has been driven by problems and challenges provided by inertial confinement fusion experiments. In recent years it has been also rapidly expanding into new areas of basic studies and applications, mainly due to dramatic new developments in a technology of ultrashort laser pulse generation and experimental conditions achieved in compression experiments of relevance to astrophysics. We are now on the brink of new developments in x-ray laser matter interactions at high radiation intensities. My research follows these new directions with studies on ultrashort pulse laser interaction with solid and gaseous targets, strongly coupled plasmas and x-ray Thomson scattering. I have also established a collaborative project in the biomedical applications of lasers. This research is focused on cytometry and cell sorting.

Sydora, R. My research in theoretical and computational plasma physics primarily concerns energy conversion and transport processes in plasmas (ionized gases) and the interrelationships between laboratory and space/astrophysical plasma environments.

• Magnetic field Reconnection, Plasmoid and Flux Rope dynamics One of the main mechanisms of energy conversion in magnetized plasmas is through a process called magnetic reconnection, a ubiquitous phenomenon in the plasma universe. In this mechanism of explosive energy release, anti-parallel magnetic field components merge and cross-connect, leading to global magnetic topology changes, plasma energization and production of high energy charged particles. To study the complex dynamics converting magnetic energy into kinetic plasma energy, we use 3D kinetic particle simulations with adaptive-mesh-refinement (AMR) to investigate the detailed microphysical processes involved. One recent important finding has been the clarification of the role of turbulence induced by plasmoids (localized magnetic bubbles) in the vicinity of the magnetic x-line where reconnection occurs and its impact on the sustainment of the reconnection process. We have identified a new form of electromagnetic turbulence leading to an enhanced or anomalous resistivity localized to the magnetic reconnection region (K. Fujimoto, R.D. Sydora, Phys. Rev. Lett., 109, 265004 (2012), image featured on issue cover)



• Particle acceleration: nonlinear plasma waves, lasers Another research theme is charged particle acceleration from coherent nonlinear plasma waves such as solitons and collisionless shocks, as well as via high-powered, tightly focused lasers in the lab. Different mechanisms produce different limits to acceleration and energy spectra; nonlinear kinetic plasma simulations are employed to test and constrain various theoretical models and design new methodologies for accelerators.

• Non-diffusive Transport in Magnetized Plasmas In more recent research, together with plasma experimentalists, we have been investigating non-diffusive transport in magnetized plasma systems that are far from equilibrium. Non-diffusive in this context means that the fundamental macroscopic parameters of a system, such as temperature and density, does not follow the standard diffusive behavior predicted by a classical Fokker-Planck equation. We have made progress in understanding how the non-diffusive properties are connected to chaotic dynamics and how this relates to exponential frequency spectra and the mathematical model of a fractional Fokker-Planck equation. From nonlinear kinetic simulations of fluctuation-driven transport in a model system (magnetized temperature filament) we have applied a permutation entropy analysis to the times series of the fluctuating electric potential and temperature in order to distinguish whether the underlying dynamics is stochastic or chaotic (eg. Lorentz or Gissinger – type). Our results indicate it is chaotic dynamics and gives insight into the nature of the turbulence.

4.8 Quantum Computation

Sanders, B.

My research lies in the area of waveguide quantum electrodynamics. My current focus areas are

- All-optical photonic switching
- Efficient quantum algorithms for quantum simulation
- Coherent electron transport in protein complexes
- Artificial intelligence for quantum control
- Quantum information processing with siliconsurface dangling bonds

- Quantum information processing with interferometry
- Modelling long-distance quantum cryptography
- Quantum coding for quantum error correction

4.9 Subatomic Physics and Field Theory

Czarnecki, A.

• New Physics searches with muonic atoms

Although most of my group's research focuses on precise predictions of the Standard Model (and developing computational techniques that make this precision possible), recently we have collaborated with an experimenter at TRIUMF, Doug Bryman, to develop a new method for searching for a "new physics" particle, the majoron. This work successfully combined our expertise in muonic atoms with Doug's knowledge of planned experiments. The method we proposed has the advantage of not requiring any changes to the future experiments, and will enrich their physics case: we pointed out how to use their results to automatically be sensitive to a new particle.

• Scattering of light on other light

The paper Photon-photon scattering earned the 2011 Best Paper Award from the Canadian Journal of Physics. The scattering of light on other light is only possible because of quantum effects known as loops (such as electron-positron pairs spontaneously created and annihilated in the vacuum; two photons can interact with such virtual particles and exchange energy). Such loop effects are somewhat tricky to evaluate and two international groups recently claimed that classic results in the literature are incorrect, not only for the photon-photon scattering but also for the Higgs decay into two photons. This latter claim was especially important because the Large Hadron Collider uses precisely this decay channel to claim the discovery of the Higgs.

Our paper resolved this dispute about the correct approach to computing loop diagrams. In addition to a mathematical proof, we included an astrophysical argument that clearly showed the error in one of the recent claims by other groups.

• Lifetime of a particle in a thermal background

All my past research focused on properties of particles in a usual vacuum, at zero temperature. There are however important applications, particularly in cosmology, of finite-temperature studies, when the vacuum is filled with black-body radiation. When the famous cosmologist, Mark Kamionkowski (Caltech/Johns Hopkins), pointed out that it is unclear how to compute particle lifetimes in such thermal background, Kirill Melnikov and I were happy to join the effort to find a solution. It turned out that our experience with loop calculations was very useful in finding the right approach. We have evaluated the leading effect of the temperature on the muon decay rate.

• Wave functions of few-body systems and extra dimensions

While it is very well known how to compute the wave function of a hydrogen atom (a two-body system), nobody knows the analytical wave function of any three-body atom. This complicates theoretical studies of helium, hydrogen ions, and other practically important systems. We were thus excited to learn from Juan Maldacena that it is possible to construct analytical solutions in the limit when the space has very many dimensions. We applied this new approach to the so-called positronium ion, a bound state of an electron and two positrons, and found excellent agreement with earlier studies by traditional methods. We thus have for the first time an alternative to numerical models employing variational methods.

Khanna, F.

Primary focus of my research has been on studies of systems at finite temperatures. This includes study of basic structure of the finite temperature theory and relationship of different theories.Applications to processes in Particle Physics,condensed matter physics and some other areas of Physics.The usual; approach is to study systems in equilibrium. Extensions to non-equilibrium processes is being considered.These include systems close to and far from equilibrium.The necessary formulation has been established and applications to specific cases is being considered.Some this work is undertaken with students from other countries.Numerous additional applications are under consideration. Additional work includes studies of Gravito-electromagnetism that include quantum version of this classical theory.At present such a Quantum theory is being considered with the inclusion of a finite temperature. A secondary interest has been to express Quantum physics in Phase space.This arose from a visit by the student a few years back .It is continuing.

Penin, A.

My recent research has led to the following results:

• New systematic effective field theory approach to describe the finite lifetime effects in the threshold production of unstable particles has been developed and applied to the top quark-antiquark pair production at LHC and ILC.

• Dominant two-loop electroweak corrections to the high-energy large-angle Bhabha scattering has been computed.

• Quantum Hall and Josephson effects remain in the focus of experimental and theoretical research over decades. The study of the effects led to development of new fundamental physical concepts. At the same time they play a crucial role in metrology and determination of fundamental constants. We have discovered a deviation from the quantum mechanical prediction for the Hall conductivity and Josephson frequency-voltage relation due to radiative antiscreening of electric charge in an external magnetic field and predicted a weak dependence of the Josephson and von Klitzing constants on the magnetic field strength. This remarkable and unexpected manifestation of a fine nonlinear quantum field effect in a collective phenomenon in condensed matter is within the reach of the existing experimental techniques and merits a dedicated experimental analysis.

4.10 Theoretical Chemical Physics

Brown, A

The interaction of light (naturally occurring or from lasers) with molecules can induce a variety of dynamical processes including electronic excitation, structural change, dissociation, and vibration. Recently, it has become possible to tailor laser fields to actively manipulate these dynamical processes. We look to develop and utilize both electronic structure and dynamical methods to understand molecular photochemistry and to manipulate molecular processes. Current projects:

Optimal control theory for laser control The use of tailored laser pulses to control chemical processes has received much attention recently, in part due to the rapid development of experimental pulse shaping techniques. We are using optimal control theory (OCT) to determine the tailored laser pulses needed to achieve control. In order to treat laser control for polyatomic molecules with more than a few (3-6) degrees of freedom, we are developing the use of the Multi-Configurational-Time-Dependent-Hartree (MCTDH) method for solving the time-dependent Schrödinger equation of the involved states in combination with OCT as well as related methods for potential energy surface fitting [4]. In related work, we are examining the use of genetic algorithms to determine the optimal laser fields for control [7,12]. The initial focus is on the study of molecular quantum computing where vibrational states represent the quantum bits (qubits) and tailored laser fields are used for implementing quantum gate operations. In order to perform the dynamics, we must determine accurate, high-dimensionality potential energy surfaces for candidate molecules for quantum computing.

Photophysics of biofluorophores We are interested in computational modeling of the photophysics of small molecules used for biological imaging [3,11]. The goal is to improve exisiting or permit the rational design of new, improved fluorescent probes.

Molecular photodissociation dynamics Molecular photofragmentation often involves multiple electronically excited and non-adiabatic transitions between these states may occur as the molecule dissociates. Our understanding of the dissociation dynamics requires both high-level theoretical calculations and the measurement of a variety of observables, particularly angular momentum distributions. We are interested in determining the complete angular momentum distributions and vector correlation coefficients (alignment and orientation) for atomic fragments resulting from molecular photofragmentation often in collaboration with experimental research groups [5,8,9]. We are also interested in developing general purpose direct dynamics (ab initio molecular dynamics) software for the study of polyatomic molecules for which quantum dynamics calculations are not feasible [12].

Hanna, G.

We have extended mixed quantum-classical methods based on the "Mixed Quantum-Classical Liouville" (MQCL) approach in order to model light-driven quantum phenomena occurring in classical environments. These methods have been applied for simulating the dynamics of two model condensed phase electron transfer reactions photo-induced by an ultrashort pump pulse. We have also developed an efficient way, based on combining the so-called equation-of-motion phase-matching approach and the aforementioned MQCL-based approaches, for calculating the time-dependent polarization of a system in any phase-matching direction in response to weak laser fields of arbitrary shape. Using this combined approach, we have simulated the pump-probe signals of the same electron transfer models and obtained decent agreement with the exact quantum results. This approach provides a general framework for calculating a host of multidimensional optical spectra.

We have taken a mixed quantum-classical approach to the simulation of the one- and two-dimensional infrared spectroscopy of hydrogen stretching modes in hydrogen-bonded system embedded in cluster, bulk, and nanoconfined environments. In particular, we have worked on bulk water, water confined in nanoscopic reverse micelles, hydrogen-bonded complexes solvated in hydrophobic cavities, and hydrogen-bonded complexes in nanoclusters of polar molecules.

We have also studied the Davydov model for energy transfer in proteins. This is a quantum mechanical model by which amide I vibrational excitations couple to alpha-helical phonon modes in such a way as to facilitate energy storage and propagation. Due to the computational expense associated with fully quantum treatments of systems with many degrees of freedom, practical solutions of this model may be obtained via mixed quantum-classical approaches. We have taken a novel mixed quantum-classical approach to this problem by implementing two methods for solving the MQCL equation, a surface-hopping solution and a second solution in which the quantum subsystem is described in terms of continuous variables. We have investigated the time-scale of vibrational delocalization in a one-dimensional Davydov model of a protein alpha helix. The results from the surface-hopping solution suggest that population transfer between distal sitesmay occur in the case of an asymmetric potential, although no transfer occurs if the vibrational excitation is treated by a mean field description.

We have taken a novel mixed quantum-classical approach to the study of proton-coupled electron transfer (PCET) reactions, which are ubiquitous in chemistry and biology. The standard surface-hopping technique has been used extensively to study PCET, but the surface-hopping solution of the MQCL equation, which more rigorously dictates the time evolution of a quantum subsystem coupled to a classical environment, has not been applied to date. More specifically, the MQCL approach naturally takes into account the contribution of quantum coherence to the dynamics, whereas the standard algorithm fails to do so. Thus, this study will give us a better understanding of the role of quantum coherence in PCET reactions. We have started implementing the MQCL-based surface-hopping algorithm on a simple model of a PCET reaction.

We have also investigated the molecular mechanisms, energetics, and kinetics of high-barrier chemical reactions and other rare events in clusters, liquids, and solids with the aid of ab-initio molecular dynamics and metadynamics. In particular, we have studied the dissociation and decomposition of carbonic acid in bulk water and water clusters and CO2 adsorption in metal organic frameworks.

We have performed simulations of the OH stretching band in the gas-phase IR spectra of strongly hydrogen-bonded dimers of phosphinic acid and their deuterated analogs, which are based on a comprehensive model for a centrosymmetric hydrogen-bonded dimer. Using a set of physically sound parameters as input into this model, we were able to successfully capture the main features in the experimental OH(D) bands. The effects of key parameters on the spectra were also elucidated.

Klobukowski, M.

We have been developing new computational methods, based on pseudopotential theory, and applied them in accurate studies of electronic structure, geometry, vibrational spectra, reaction mechanisms, and one-electron properties of organometallic molecules, molecular ions, and molecular clusters in their ground and excited electronic states. We have been interested in both small and large molecules: we study systems from atoms to proteins.

More specifically, we have been interested in:

• Development, calibration, and applications of pseudopotential methods required to deal with large molecules or molecular systems containing heavy atoms; our model core potentials allow for the description of the scalar relativistic effects.

• Development and applications of methods to calculate both 1- and 2-electron spin-orbit effects.

• Development of basis sets for all-electron relativistic calculations on molecules containing very heavy atoms.

• Molecular structure and properties of very large molecules and molecular clusters using both nonrelativistic and scalar-relativistic model core potential representation of the core electrons and correlated wavefunctions or density functionals for the description of the valence electrons. We are particularly interested in the interactions of such systems with metal ions.

• Weakly bonded systems containing noble gas atoms in ground end excited electronic states, especially novel compounds that contain noble-gas elements.

• Design of novel anti-cancer drugs. In this case, in order to be able to represent both the drug molecule as well as the target protein, we use the hybrid QM/MM approach, with the quantum mechanical treatment used for the drug molecule, and molecular mechanics used to model protein.

Roy, P.-N.

Quantum Molecular Dynamics: Atoms and Molecules in Motion

Our research is aimed at the understanding of the dynamics of complex molecular systems. To this end, we are developing theoretical approaches and numerical algorithms for computer simulations. We are interested in various levels of theory from classical molecular dynamics and Monte Carlo approaches for the simulation of large biomolecular systems, to extreme quantum mechanical situations where both dispersion and quantum statistical effects have to be accounted for, such as in the case of quantum clusters and fluids. We are also developing semi-classical approaches for intermediate cases where a classical description fails but where an approximate quantum mechanical treatment is sufficient to capture the relevant phenomenology.

Current Research Topics include:

• Formal developments of the Feynman Path centroid approach for systems obeying Bose-Einstein statistics.

• Path Integral simulations of quantum fluids.

• Simulations of doped helium nano-droplets.

• Exact Quantum Dynamics of weakly bound clusters.

• Molecular Dynamics simulation of Protein-ligand systems in solution and in the gas phase.

• Dynamics of hydrogen bonded complexes and proton transfer.

• Development of semi-classical quantum dynamics approaches.

5 International collaborations

At the international level TPI has spearheaded several collaborative agreements that serve as the basis for collaboration between University of Alberta researchers and their foreign counterparts. These long term agreements are with

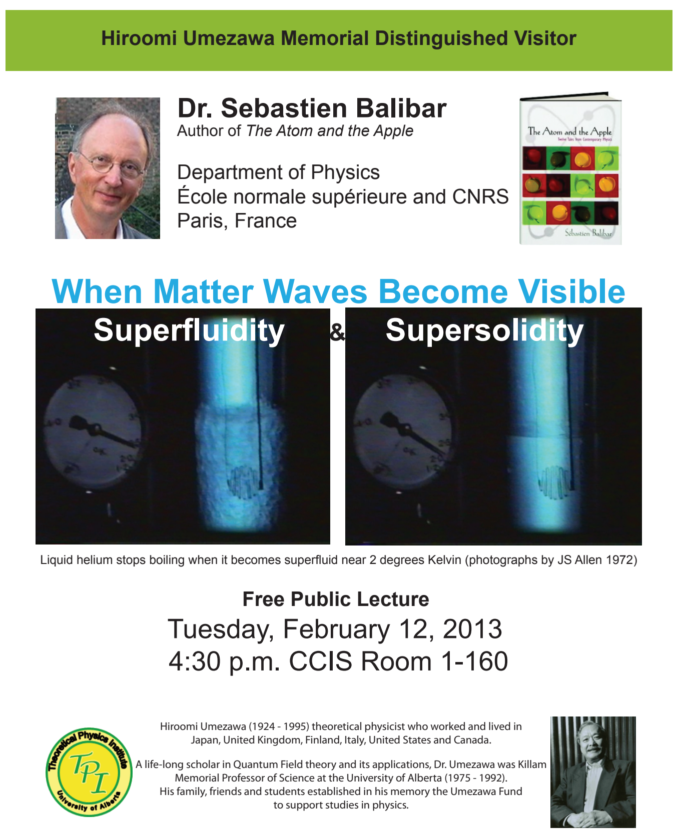
- Pacific Center of Theoretical Physics (APCTP, Korea),
- Kunsan National University (Korea).
- Yukawa Institute for Theoretical Physics (University of Kyoto),
- Recently TPI initiated the MOU between the Faculty of Science and the Faculty of Physics and Mathematics of the Charles University (Prague, Czech Republic) that has been successfully signed in May 2013.

6 International Visitor Program

6.1 Hiromi Umezawa Distinguished Lectureship

In February 2013, Dr. Sebastien Balibar, CNRS director of research at the Laboratoire de Physique Statistique at l'Ecole Normale Superieure in Paris, Fellow of the American Physical Society and member of the French Academy of Science, was our Distinguished Umezawa Lecturer.

Dr. Balibar is a preeminent experimentalist in the low temperature physics, who has been awarded all major honors in the field including the London Prize for Low Temperature Physics. He gave two lectures at the University of Alberta. The first, public one was titled "When matter waves become visible" and was an elegant discourse into the history of research superfluidity, supported by original and striking visual demonstrations of superfluidity in Helium-3 that captivated the audience. The second, physics colloquium, was on the topic of "The giant plasticity of a quantum crystal" which discussed newly discovered phenomena in ultra-pure low temperature Helium-4 that exhibits almost no resistance to shear in some directions.

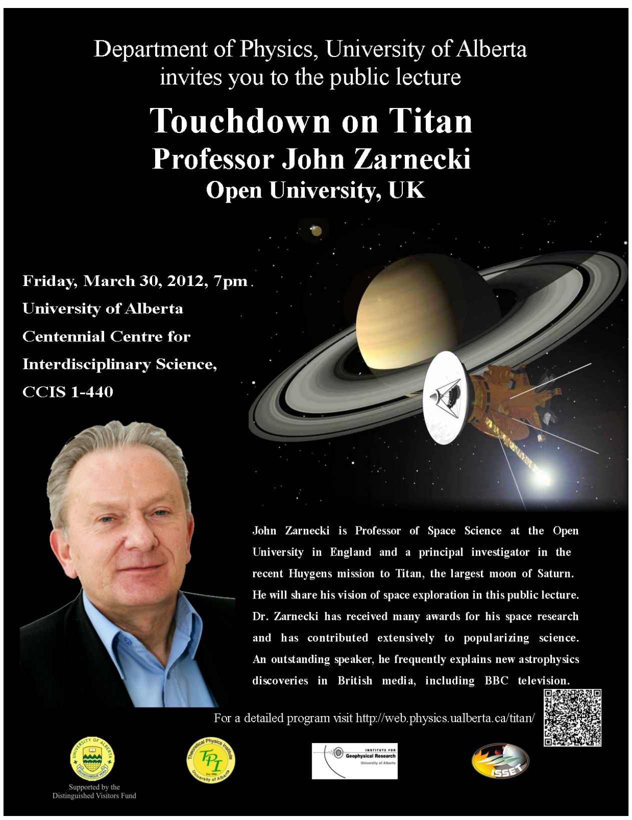


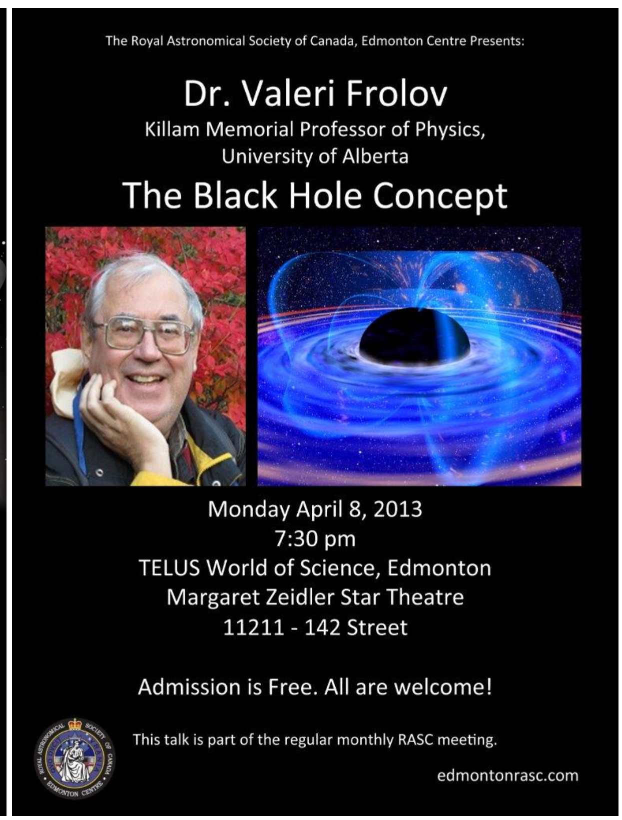
6.2 Public Presentations

In March 2012, TPI was fortunate to host Prof. John Zarnecki who visited University of Alberta as a recipient of the Distinguished Visitor Award from the Faculty of Science. Professor John Zarnecki, Professor of Space Science at the Open University, brought to share with us his experience of over 30 years of world-leading space research, including some of the most iconic unmanned space programmes ever undertaken. These include developing instrumentation for the Hubble Space Telescope, Europe's Giotto mission which successfully flew past Halley's comet in 1985, and the recent NASA/ESA (European Space Agency) mission to the Saturnian system. He has contributed extensively to popularizing science. In addition to his research and outreach activities, he is active in various top level advisory groups such the UK's Space Leadership Council and the ESA's Human Exploration and Science Advisory Committee.

In April 2013, our own Prof. V. Frolov, by invitation of the Royal Astronomical Society of Canada (Edmonton Centre), introduced to the public "The Black Hole Concept".

Both events served as a great benefit to science-minded public at our University and the City of Edmonton and showcased the fascinating scientific advances achieved right here at home and by the scientific community at large.





6.3 TPI seminars series

TPI continues to maintain an active visitor and seminar program. This is one of the prime focus of the Institute activities aimed at facilitating collaborations in the field of theoretical physics within University of Alberta, Canada as a whole and internationally. TPI seminar series is a prime vehicle of continuing enhancement of the Institute recognition in the scientific community. In the last two years TPI has initiated and/or facilitated the following visits and presentations.

- Prof. M. Revzen (Technion, Israel): "Classical and Quantum State Reconstruction", Aug. 29th, 2011
- Dr. Edward Rietman (Center of Cancer Systems Biology, St. Elizabeths Medical Center, Tufts University School of Medicine): "Genomes, Dandelions and Galaxies: Molecular Systems Biology in the Real World", September 8th, 2011
- Dr. Massimo Pregnolato (University of Pavia, Italy): "Analysis of the EPR spectra of Microtubules and computational studies of their interactions with drugs", November 3rd, 2011
- Dr. David Morrissey (TRIUMF): "The Matter with Antimatter", March 13th, 2012
- Prof. John Zarnecki (Open University, UK): "Europe's Cometary Space Missions, Past and Present: from Giotto to Rosetta", April 2nd, 2012
- Dr. V. I. Korobov (Joint Institute for Nuclear Research, Dubna, Russia): "Precision spectroscopy, fundamental physical constants, and SI units", April 4th, 2012
- Dr. Chris Done (Durham Univ): "Using stellar mass black holes to understand AGN", July 3rd, 2012
- Dr. Cecilia Flori (Perimeter Institute): "Topos Formulation of Quantum Theory", Sept. 6th, 2012
- Prof. Bill Unruh (UBC): "Decoherence and energy conservation", Sept. 13th, 2012
- Dr. Richard Hill (University of Chicago and Enrico Fermi Institute): "Heavy Particle Effective Field Theory: Formalism and new applications to atoms and dark matter", September 26th, 2012
- Prof. Sebastien Balibar (Ecole Normale Superieure and CNRS, France): "The giant plasticity of a quantum crystal", February 14th, 2013
- Dr. Cesare Tronci (University of Surrey, UK): "Geometry and symmetry in multi-physics models for magnetized plasmas", March 8th, 2013, Joint AMI/TPI
- Prof. Douglas Scott (UBC): "New results from Planck: A more precise Universe", April 12th, 2013
- Dr. Matt Dowling (DESY) "High Order Corrections to Heavy to Light Decays", June 10, 2013

6.4 Long-term visitors

During the reported period TPI has welcomed and supported several long-term visitors, who has stayed at affiliated departments for longer than two weeks. This list comprises of:

- Prof. M. Revzen (Technion, Israel)
- Dr. Edward Rietman (Tufts University)
- Archisman Ghosh (University of Kentucky)
- Dr. Adolfo Malbouisson (CBPF,BRazil)
- Dr. Jorge Malbouisson (Salvador,Brazil)
- Dr. Ademir Santana (Brasilia,Brazil).
- Dr. Christophe Pichon (IAP, France)
- Dr. Christophe Gay (IAP, France)
- Sandrine Codis (IAP, France)
- Prof. Valeri Bychenkov (Lebedev Physics Institute, Moscow)

7 Conferences and meetings

Among conference activities TPI was at the root of highly successful series of international meetings “Black Holes”, with the first “Black Hole I” organized by TPI in Banff in 1997. The series is held by-annually, with every odd one organized by TPI. Exception was “Black Holes IX” conference in May 2013, which organization was delegated to University of Saskatchewan. This series has high international stature attracting top scientists from around the world and TPI is looking forward to return its organization to Alberta in 2015.

In the last two years another meeting that TPI has supported is “Theory Canada VII”, a satellite conference to CAP congress, held in Lethbridge in June 2012.

Members of the institute took part in organization of several international conferences, among them

• International 5 day workshop ”Black Holes: New Horizons” (11w5099), November 2011, Banff (V. Frolov and D. Page, organizers)

• Conference “Challenges for Early Universe cosmology“, (Perimeter Institute), July 2011, (D. Page, member of International Organizing Committee)

• XIV International Conference ”Geometry, Integrability and Quantization” , Varna, Bulgaria, June 2012 (V. Frolov, member of Advisory Committee)

• ”Relativity and Gravitation: 100 Years after Einstein in Prague”, June, 2012 (V. Frolov, member of Organizing Committee)

• International program “Common Envelope” Kavli Institute for Astronomy & Astrophysics, Beijing, China, March-April 2011 (N. Ivanova, member of Scientific Organizing Committee)

• CASCA, Canadian Astronomy Society Annual Meeting - 2011 London, Ontario, May 2011, (N. Ivanova, member of Scientific Organizing Committee)

• Jan 2012, “The Physics of Astronomical Transients” Conference, the Aspen Center for Physics, Aspen, USA, Jan 2012, member of Scientific Organizing Committee)

• XV International Conference ”Geometry, Integrability and Quantization”, Varna, Bulgaria, June 2013 (V. Frolov, member of Advisory Committee)

• XI-th International Conference on Gravitation, Astrophysics and Cosmology of Asia-Pacific Countries (Kazakh National University), October 2013, (V. Frolov, member of Advisory Committee)

• International meeting ”Black and Dark Topics of Modern Cosmology and Astrophysics”, (Dubna, Russia) September 2013 (V. Frolov, member of Advisory Committee)

• International colloquium “Origin of the Hubble sequence” (IAP 75th anniversary), (Paris, France), June 2013 (D. Pogosyan, member of both Local and Scientific Organizing Committees)

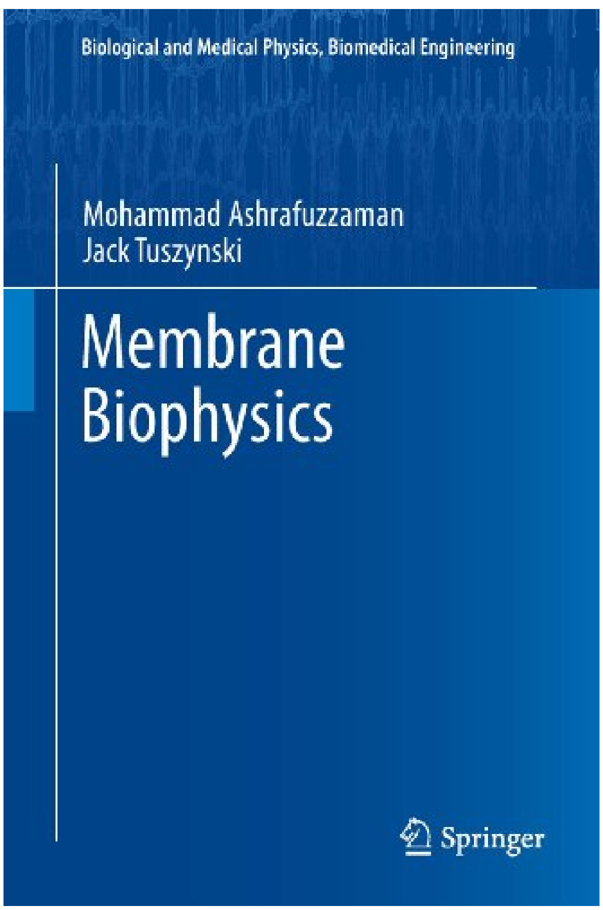
8 Publications

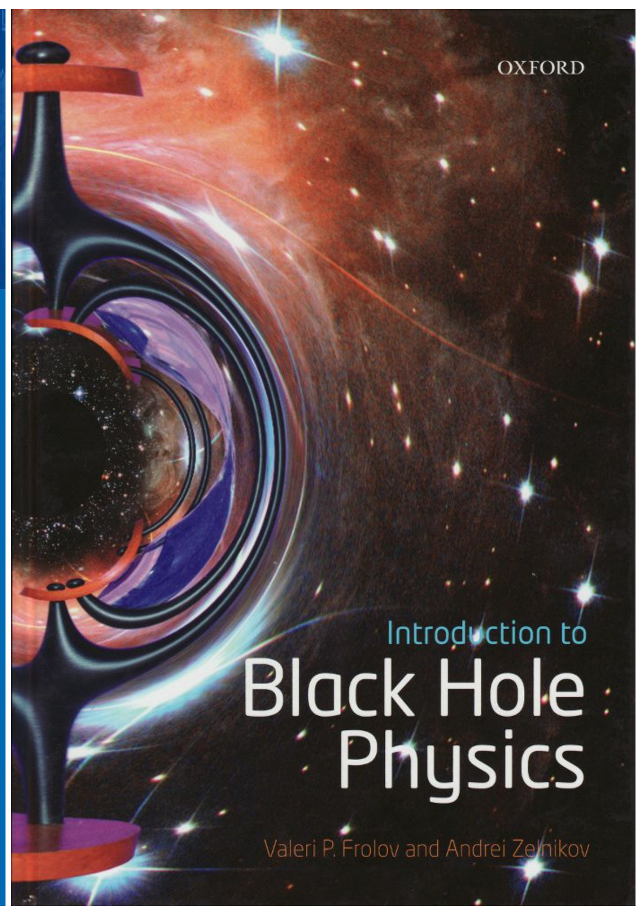
8.1 Books

Members of TPI have written two monographs

- “Membrane biophysics” by Mohammad Ashrafuzzaman and Jack Tuszynski, published by Springer.

- “Introduction to Black Hole Physics” by Valeri Frolov and Andrei Zelnikov, published by Oxford University Press.





8.2 Refereed Contributions

1. Experimental and Computational Study of the Interaction of Novel Colchicinoids with a Recombinant Human αI/βI-Tubulin Heterodimer JY Mane, V Semenchenko, R Perez-Pineiro, P Winter, D Wishart, **JA Tuszynski** Chemical biology & drug design 82 (1), 60-70, (2013)

2. An integrated multidisciplinary model describing initiation of cancer and the Warburg hypothesis EA Rietman, DE Friesen, P Hahnfeldt, R Gatenby, L Hlatky, **JA Tuszynski** Theoretical Biology and Medical Modelling 10 (1), 39, (2013)

3. Determination of the optimal tubulin isotype target as a method for the development of individualized cancer chemotherapy S Ravanbakhsh, M Gajewski, R Greiner, **JA Tuszynski** Theoretical Biology and Medical Modelling 10 (1), 29, (2013)

4. Interactions of laulimalide, peloruside, and their derivatives with the isoforms of β-tubulin MM Gajewski, **JA Tuszynski**, K Barakat, JT Huzil, M Klobukowski Canadian Journal of Chemistry 91 (7), 511-517, (2013)

5. Dynamic Change of Heme Environment in Soluble Guanylate Cyclase and Complexation of NOIndependent Drug Agents with H-NOX Domain L Alisaraie, Y Fu, **JA Tuszynski** Chemical biology & drug design 81 (3), 359-381, (2013)

6. Stochastic and deterministic models of cellular p53 regulation GB Leenders, **JA Tuszynski** Frontiers in oncology 3,(2013)

7. Lipid Membrane Binding of Computationally-Designed DNA Aptamers Specific for Phosphatidylserine M Ashrafuzzaman, HM Embark, HB Jagirdar, A Alsenaidy, CY Tseng, **JA Tuszynski** Biophysical Journal 104, 93, (2013)

8. Saturable Fractal Pharmacokinetics and Its Applications RE Marsh, **JA Tuszynski** Mathematical Methods and Models in Biomedicine, 339-366,(2013)

9. The Membrane as a Transporter, Ion Channels and Membrane Pumps M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 51-74, (2013)

10. Membrane-Related Diseases, M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 151-170, (2013)

11. Lipids in Membranes, M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 31-49, (2013)

12. Structure of Membranes, M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 9-30, (2013)

13. Membrane-Based Nanotechnology and Drug Delivery, M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 127-149, (2013)

14. Lipid Bilayer-Membrane Protein Coupling, M Ashrafuzzaman, **J Tuszynski** Membrane Biophysics, 75-125, (2013)

15. Activation of Hydrogen Peroxide to Peroxytetradecanoic Acid Is Responsible for Potent Inhibition of Protein Tyrosine Phosphatase CD45 A Kuban-Jankowska, **JA Tuszynski**, P Winter, M Gorska, N Knap, M Wozniak PloS one 7 (12), e52495

16. Virtual screening and biological evaluation of inhibitors targeting the XPA-ERCC1 interaction KH Barakat, LP Jordheim, R Perez-Pineiro, D Wishart, C Dumontet, **JA Tuszynski** PloS one 7 (12), e51329, (2012)

17. Chemotherapy drugs form ion pores in membranes due to physical interactions with lipids M Ashrafuzzaman, CY Tseng, M Duszyk, **JA Tuszynski** Chemical Biology & Drug Design 80 (6), 992-1002, (2012)

18. Self-organization and entropy reduction in a living cell PCW Davies, E Rieper, **JA Tuszynski** Biosystems 1, (2012)

19. Modeling the Yew Tree Tubulin and a Comparison of its Interaction with Paclitaxel to Human Tubulin, **JA Tuszynski**, TJA Craddock, JY Mane, K Barakat, CY Tseng, M Gajewski, P ... Pharmaceutical research 29 (11), 3007-3021, (2012)

20. Peloruside, Laulimalide, and Noscapine Interactions with Beta-Tubulin, MM Gajewski, L Alisaraie, **JA Tuszynski** Pharmaceutical research 29 (11), 2985-2993, (2012)

21. Simulation of the effects of microtubules in the cortical rotation of amphibian embryos in normal and zero gravity, C Nouri, **JA Tuszynski**, MW Wiebe, R Gordon Biosystems 109 (3), 444-449, (2012)

22. A mean field Ising model for cortical rotation in amphibian one-cell stage embryos, **JA Tuszynski**, R Gordon Biosystems 109 (3), 381-389, 2012

23. DNA polymerase beta (pol β) inhibitors: A comprehensive overview, KH Barakat, MM Gajewski, **JA Tuszynski** Drug discovery today 17 (15), 913-920, (2012)

24. Dissipationless Transfer of Visual Information from Retina to the Primary Visual Cortex in the Human Brain, VS Salari, M Rahnama, **JA Tuszynski** ANS: The Journal for Neurocognitive Research 54 (1-2), (2012)

25. Computational predictions of volatile anesthetic interactions with the microtubule cytoskeleton: implications for side effects of general anesthesia TJA Craddock, MS George, H Freedman, KH Barakat, S Damaraju, S Hameroff, **JA Tuszynski** ... PloS one 7 (6), e37251, (2012)

26. Molecular signaling network complexity is correlated with cancer patient survivability D Breitkreutz, L Hlatky, E Rietman, **JA Tuszynski** Proceedings of the National Academy of Sciences 109 (23), 9209-9212, (2012)

27. SAR-3419. Antibody-drug immunoconjugate, Oncolytic **JA Tuszynski**, DRUGS OF THE FUTURE 37 (6), 419-422, (2012)

28. The Molecular Mechanism of Action of the CR6261-Azichromycin Combination Found through Computational Analysis W Cui, K Wang, J Ruan, Z Qi, Y Feng, Y Shao, **JA Tuszynski** PloS one 7 (5), e37790, (2012)

29. Ion pore formation in lipid bilayers and related energetic considerations, M Ashrafuzzaman, **J Tuszynski** Current medicinal chemistry 19 (11), 1619-1634, (2012)

30. Regulation of channel function due to coupling with a lipid bilayer, M Ashrafuzzaman, **J Tuszynski** Journal of Computational and Theoretical Nanoscience 9 (4), 564-570, (2012)

31. Synthesis and evaluation of fluorobenzoylated di-and tripeptides as inhibitors of cyclooxygenase-2 (COX-2) SK Sharma, BJ Al-Hourani, M Wuest, JY Mane, **J Tuszynski**, V Baracos, M Suresh ... Bioorganic & medicinal chemistry 20 (7), 2221-2226, (2012)

32. The zinc dyshomeostasis hypothesis of Alzheimer's disease TJA Craddock, **JA Tuszynski**, D Chopra, N Casey, LE Goldstein, SR Hameroff, RE ... PloS one 7 (3), e33552, (2012)

33. Implications of quantum metabolism and natural selection for the origin of cancer cells and tumor progression, P Davies, LA Demetrius, **JA Tuszynski** AIP advances 2 (1), 011101-011101-14, (2012)

34. Cytoskeletal signaling: is memory encoded in microtubule lattices by CaMKII phosphorylation?, TJA Craddock, **JA Tuszynski**, S Hameroff PLoS computational biology 8 (3), e1002421, (2012)

35. An investigation of the plausibility of stochastic resonance in tubulin dimers, AA Saha, TJA Craddock, **JA Tuszynski** Biosystems 107 (2), 81-87, (2012)

36. Meyer-Overton meets quantum physics: conscious awareness, memory, and anaesthetic binding in tubulin hydrophobic channels, S Hameroff, T Craddock, **J Tuszynski** BRITISH JOURNAL OF ANAESTHESIA 108 (2), 341P-342P, 2012

37. A Theoretical Estimation for Dipole Moment Direction of Tubulin Dimer and Assessment of Microtubule Folding Possibility, A Samarbakhsh, **J Tuszynski** Biophysical Journal 102 (3), 698a, (2012)

38. Computational and Theoretical Nanoscience, J Yuan, Y Chen, Y Mao, B Liao, T Cao, X Lu, W Zhu, J Luo, H He, J Yan, C He ... J. Comput. Theor. Nanosci 9, 2265-2279, (2012)

39. Resonance Condition in Microtubules Using Ultrasound Plane Waves, A Samarbakhsh, **J Tuszynski** Journal of Computational and Theoretical Nanoscience 9 (1), 67-71, (2012)

40. Xiaoming Zhang and **K. S. D. Beach**, "Resonating valence bond trial wave functions with both static and dynamically determined Marshall sign structure," Physical Review B 87, 094420 (2013).

41. T. S. Biswas, A. Suhel, B. D. Hauer, A. Palomino, **K. S. D. Beach**, J. P. Davis, "High-Q Gold and Silicon Nitride Bilayer Nanostrings," Applied Physics Letters 101, 093105 (2012).

42. A. Suhel, B. D. Hauer, T. S. Biswas, **K. S. D. Beach**, J. P. Davis, Dissipation Mechanisms in Thermomechanically Driven Silicon Nitride Nanostrings, Applied Physics Letters 100, 173111 (2012).

43. **K. S. D. Beach** and F. F. Assaad, "Orbital-selective Mott transition and heavy-fermion behavior in a bilayer Hubbard model for 3He," Physical Review B 83, 045103 (2011).

44. Perturbation theory of the mass enhancement for a polaron coupled to acoustic phonons Z. Li, C.J. Chandler, and **F. Marsiglio** Phys. Rev. B 83, 045104 (2011).

45. The static electric polarizability of a particle bound by a finite potential well M.A. Maize, M.A. Antonacci, and **F. Marsiglio** American Journal of Physics 79, 222 (2011).

46. Electron-hole asymmetry in the Dynamic Hubbard model G.H. Bach and **F. Marsiglio** J. Superconductivity and Novel Magnetism 24, 1571-1575, (2011).

47. Impact of spin-orbit coupling on the Holstein polaron Zhou Li, L. Covaci, M. Berciu, D. Baillie, and **F. Marsiglio** Phys. Rev. B83, 195104 (2011).

48. Surface effects in doping a Mott insulator Reza Nourafkan and **Frank Marsiglio** Phys. Rev. B83, 155116 (2011).

49. Microcavity effects in ensembles of silicon quantum dots coupled to high-Q resonators P. Bianucci, Y.Y. Zhi, **F. Marsiglio**, J. Silverstone, and A. Meldrum Physica Status Solidi A208, 639 (2011).

50. Competition between reduced delocalization and charge transfer effects for a two-band Hubbard model R. Nourafkan and **F. Marsiglio** Phys. Rev. B84, 075133 (2011).

51. 'Conventional' Superconductivity: A Critical Assessment **F. Marsiglio** Physics in Canada 67,71 (2011).

52. Optical conductivity for a dimer in the dynamic Hubbard model G.H. Bach and **F. Marsiglio** Phys. Rev. B85, 155134 (2012).

53. Impact of Dresselhaus versus Rashba spin-orbit coupling on the Holstein polaron, Zhou Li, L. Covaci and **F. Marsiglio** Phys. Rev. B85, 205112 (2012).

54. The Polaron-Like Nature of an Electron Coupled to Phonons, Zhou Li and **F. Marsiglio** JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM 25, 1313 (2012).

55. Model of the Electron-Phonon Interaction and Optical Conductivity of $Ba_{1-x}K_xBiO_3$ Superconductors, R. Nourafkan, **F. Marsiglio** and G. Kotliar Phys. Rev. Lett. 109 017001 (2012)

56. The superconducting (BCS) pairing instability in the thermodynamic limit, **F. Marsiglio, K.S.D. Beach**, and R.J. Gooding Can. J. Phys. 90, 889 (2012)

57. The double well potential in quantum mechanics: a simple, numerically exact formulation, V. Jelic and **F. Marsiglio** Eur. J. Phys. 33 1651 (2012).

58. The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals Joel Hutchinson, Marc Baker and **F. Marsiglio** Eur. J. Phys. 34 111 (2013).

59. The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals, B.A. Jugdutt and **F. Marsiglio** Am. J. Phys. 81, 343 (2013).

60. Self-energy anomaly of an electric pointlike dipole in three-dimensional static spacetimes, **Valeri P. Frolov**, Andrey A. Shoom, **Andrei Zelnikov**. Mar 7, 2013. 7 pp. ALBERTA-THY-02-13 (accepted for publication Phys.Rev.D) e-Print: arXiv:1303.1816 [gr-qc]

61. Critical escape velocity for a charged particle moving around a weakly magnetized Schwarzschild black hole, A.M.Al Zahrani, **Valeri P. Frolov**, Andrey A. Shoom. Jan 2013, Phys.Rev. D87 (2013) 084043

62. Electron in higher-dimensional weakly charged rotating black hole spacetimes, Marco Cariglia, **Valeri P. Frolov**, Pavel Krtous, David Kubiznak. Nov 2012, Phys.Rev. D87 (2013) 064003

63. Geometry of Lax pairs: particle motion and Killing-Yano tensors Marco Cariglia, **Valeri P. Frolov**, Pavel Krtous, David Kubiznak. Oct 2012, Phys.Rev. D87 (2013) 024002

64. **Valeri P. Frolov**, Andrey A. Shoom, (2012) “Scattering of circularly polarized light by a rotating black hole”, Phys.Rev.D 86, 024010

65. **Valeri P. Frolov**, (2012) “Weakly magnetized black holes as particle accelerators”, Phys.Rev. D85, 024020

66. **Valeri P. Frolov**, Andrey A. Shoom, (2011) “Spinoptics in a stationary spacetime”, Phys.Rev.D 84, 044026

67. **Valeri P. Frolov** and Shinji Mukohyama, (2011) “Brane Holes”, Phys. Rev. D83, 044052

68. Valeri P. Frolov and Pavel Krtous, (2011) “Charged particle in higher dimensional weakly charged rotating black hole spacetime.” Phys. Rev. D83, 024016

69. A.M. Al Zahrani, **Valeri P. Frolov**, Andrey A. Shoom, (2011) “Particle Dynamics in Weakly Charged Extreme Kerr Throat”, Int.J.Mod.Phys. D20, 649-660

70. Heinke, C. O., **Ivanova, N.**, Engel, M. C., et al. 2013, ApJ, 768, 184

71. Cartwright, T. F., Engel, M. C., Heinke, C. O., et al. 2013, ApJ, 768, 183

72. Pavlovskii, K., & **Ivanova, N.** 2013, IAU Symposium, 291, 468

73. Pavlovskii, K., & **Ivanova, N.** 2013, IAU Symposium, 290, 293

74. Kim, D.-W., Fabbiano, G., **Ivanova, N.**, et al. 2013, ApJ, 764, 98

75. **Ivanova, N.**, Justham, S., Chen, X., et al. 2013, A&ARv, 21, 59

76. **Ivanova, N.**, Justham, S., Avendano Nandez, J. L., & Lombardi, J. C. 2013, Science, 339, 433

77. **Ivanova, N.** 2013, Memorie della Societa Astronomica Italiana, 84, 123

78. **Ivanova, N.**, Fragos, T., Kim, D.-W., et al. 2012, ApJ, 760, L24

79. "The Large Observatory for X-ray Timing (LOFT)", Feroci, M., Stella, L., van der Klis, M., et al. 2012, Experimental Astronomy, 34, 415

80. "LOFT: the Large Observatory For X-ray Timing", Feroci, M., den Herder, J. W., Bozzo, E., et al. 2012, Proceedings of SPIE, 8443.

81. "Constraints on the Mass and Radius of the Neutron Star XTE J1807-294", Leahy, D. A., **Morsink, S. M.**, & Chou, Y. 2011, ApJ, 742, 17

82. "Multi-epoch Analysis of Pulse Shapes from the Neutron Star SAX J1808.4-3658" **Morsink, S. M.**, & Leahy, D. A. 2011, ApJ, 726, 56

83. Scalar-tensor gravitation and the Bakry-Émery-Ricci tensor, **E Woolgar**, Class Quantum Gravit 30 (2013) 085007

84. The Ricci flow of asymptotically hyperbolic mass and applications, T Balehowsky and **E Woolgar**, J Math Phys 53 (2012) 072501

85. **Don N. Page**, "Agnesi Weighting for the Measure Problem of Cosmology," J. Cosmol. Astropart. Phys., 1103, 031-0–031-18 (2011)

86. **Don N. Page**, "Statistical Evidence Against Simple Forms of Wavefunction Collapse," Phys. Lett. B, 719, 207-209 (2013)

87. **Don N. Page**, "Preliminary Inconclusive Hint of Evidence Against Optimal Fine Tuning of the Cosmological Constant for Maximizing the Fraction of Baryons Becoming Life" (University of Alberta report Alberta-Thy-02-11, January 2011), arXiv:1101.2444 [hep-th]

88. **Don N. Page**, "Consciousness and the Quantum," J. Cosmology, 14, arXiv:1102.5339

89. **Don N. Page**, "Finite Canonical Measure for Nonsingular Cosmologies," J. Cosmol. Astropart. Phys., 1106, 038-0–038-16 (2011)

90. **Don N. Page**, "Ab Initio Estimates of the Size of the Observable Universe," J. Cosmol. Astropart. Phys., 1109, 037-0–037-6 (2011)

91. **Don N. Page**, "The Superb Design," in Faith Seeking Understanding: Essays in Memory of Paul Brand and Ralph D. Winter, edited by David Marshall (William Carey Library, Pasadena, California, 2012), pp. 179-190.

92. **Don N. Page**, "Does God Love the Multiverse?" in The Blackwell Companion to Science and Christianity, edited by J. B. Stump and Alan G. Padgett (Wiley, Malden, Massachusetts, 2012), pp. 198-206.

93. **Don N. Page**, "Quantum Uncertainties in the Schmidt Basis Given by Decoherence," arXiv:1108.2709

94. **Don N. Page**, "Normalized Observational Probabilities from Unnormalizable Quantum States or Phase-Space Distributions," arXiv:1203.1837

95. **Don N. Page** and Xing Wu, "Massless Scalar Field Vacuum in de Sitter Spacetime," J. Cosmol. Astropart. Phys., 1211, 051-0–051-16 (2012)

96. Shohreh Abdolrahimi, Celine Cattoen, **Don N. Page**, and Shima Yaghoobpour-Tari, "Large Randall-Sundrum II Black Holes," Phys. Lett. B, 720, 405-409 (2013)

97. **Don N. Page**, "Generalized Jarzynski Equality," arXiv:1207.3355 [hep-th]

98. **Don N. Page**, "Hyper-Entropic Gravitational Fireballs (Grireballs) with Firewalls ," J. Cosmol. Astropart. Phys., 1304, 037-0–037-14 (2013)

99. Shohreh Abdolrahimi, Celine Cattoen, **Don N. Page**, and Shima Yaghoobpour-Tari, "S pectral Methods in General Relativity and Large Randall-Sundrum II Black Holes," J. Cosmo l. Astropart. Phys., 1306, 039-0–039-24 (2013)

100. Sang Pyo Kim and **Don N. Page**, "Exact Quantum Statistical Dynamics of Time Dependent Generalized Oscillators," Phys. Lett. B, 723, 393-396 (2013)

101. **Don N. Page**, "Time Dependence of Hawking Radiation Entropy," arXiv:1301.4995

102. **Don N. Page**, "Excluding Black Hole Firewalls with Extreme Cosmic Censorship," arXiv:1306.0562

103. Non-Gaussian Minkowski functionals & extrema counts in redshift space S Codis, C Pichon, **D Pogosyan**, F Bernardeau, T Matsubara arXiv preprint arXiv:1305.7402 (accepted to MNRAS, July 2013)

104. Planck 2013 results. XXIII. Isotropy and Statistics of the CMB PAR Ade, N Aghanim, C Armitage-Caplan, M Arnaud, M Ashdown, F Atrio ... arXiv preprint arXiv:1303.5083, (2013)

105. Planck 2013 results. XXVI. Background geometry and topology of the Universe P Collaboration, PAR Ade, N Aghanim, C Armitage-Caplan, M Arnaud, M Ashdown ... arXiv preprint arXiv:1303.5086, (2013)

106. Connecting the cosmic web to the spin of dark halos: implications for galaxy formation, S Codis, C Pichon, J Devriendt, A Slyz, **D Pogosyan**, Y Dubois, T Sousbie Monthly Notices of the Royal Astronomical Society 427 (4), 3320-3336, (2012)

107. Non Gaussianity and Minkowski Functionals: forecasts for Planck A Ducout, F Bouchet, S Colombi, **D Pogosyan**, S Prunet MNRAS, 429, 3, 2104-2126, (2013)

108. Feeding compact bulges and supermassive black holes with low angular momentum cosmic gas at high redshift, Y Dubois, C Pichon, M Haehnelt, T Kimm, A Slyz, J Devriendt, **D Pogosyan** Monthly Notices of the Royal Astronomical Society 423 (4), 3616-3630, (2012)

109. Statistical Description of Synchrotron Intensity Fluctuations: Studies of Astrophysical Magnetic Turbulence, A Lazarian, **D Pogosyan** The Astrophysical Journal 747 (1), 5, (2012)

110. Non-Gaussian statistics of critical sets in 2D and 3D: Peaks, voids, saddles, genus, and skeleton, C Gay, C Pichon, **D Pogosyan** Physical Review D 85 (2), 023011, (2012)

111. Rigging dark haloes: why is hierarchical galaxy formation consistent with the inside-out build-up of thin discs? C Pichon, **D Pogosyan**, T Kimm, A Slyz, J Devriendt, Y Dubois Monthly Notices of the Royal Astronomical Society 418 (4), 2493-2507, (2011)

112. Non-Gaussian extrema counts for CMB maps **D Pogosyan**, C Pichon, C Gay Physical Review D 84 (8), 083510, (2011)

113. Anomaly and the self-energy of electric charges, **VP Frolov, A Zelnikov** Physical Review D 86 (10), 104021, (2012)

114. Higher-dimensional Kundt waves and gyratons, P Krtous, J Podolský, **A Zelnikov**, H Kadlecová Physical Review D 86 (4), 044039, (2012)

115. Classical self-energy and anomaly, **VP Frolov, A Zelnikov** Physical Review D 86 (4), 044022, (2012)

116. Self-energy of a scalar charge near higher-dimensional black holes, **VP Frolov, A Zelnikov** Physical Review D 85 (12), 124042, (2012)

117. Scalar and electromagnetic fields of static sources in higher dimensional Majumdar-Papapetrou spacetimes **VP Frolov, A Zelnikov** Physical Review D 85 (6), 064032, (2012)

118. Casimir Cascades in Two-Dimensional Turbulence, **J. C. Bowman**, Journal of Fluid Mechanics, (2013).

119. Multithreaded Implicitly Dealiased Pseudospectral Convolutions, M. Roberts and **J. C. Bowman**, Proceedings of the 20th Annual Conference of the CFD Society of Canada, (2012).

120. Pseudospectral Reduction of Incompressible Two-Dimensional Turbulence, **J. C. Bowman** and M. Roberts, Communications in Nonlinear Science and Numerical Simulation, 17:5, 2008-2013 (2012).

121. Surface Parameterization of Nonsimply Connected Planar Bzier Regions, O. Shardt and **J. C. Bowman**, Computer-Aided Design, 44:5, 484.e1-10 (2012)

122. Dealiased Convolutions for Pseudospectral Simulations, M. Roberts and **J. C. Bowman**, Journal of Physics: Conference Series,318:7, 072037, 1-6 (2011)

123. Efficient Dealiased Convolutions without Padding, **J. C. Bowman** and M. Roberts, SIAM Journal on Scientific Computing, 33:1, 386-406 (2011)

124. "Samples of noncommutative products in certain differential equations", **M. Légaré**, Journal of Physics A : Math. Theor. 43, (44), 445208, 2010, (14 pp).

125. "Certain non-commuting variables, n-ary algebras, and first-order differential equations", **M. Légaré**, preprint, Dec. 2012, (22 pp).

126. V. Brantov, V. Yu. Bychenkov and **W. Rozmus**, Electrostatic response of a two-component plasma with Coulomb collisions, Phys. Rev. Letters 108, 205001 (2012)

127. T. Chapman, S. Huller, P.-E. Masson-Laborde, A. Heron, D. Pesme, **W. Rozmus**, Driven Spatially Autoresonant Stimulated Raman Scattering in the Kinetic Regime, Phys. Rev. Letters 108, 145003 (2012)

128. P.-E. Masson-Laborde, **W. Rozmus**, Z. Peng, D. Pesme, S. Huller, M. Casanova, V. Yu. Bychenkov, T. Chapman, and P. Loiseau, Evolution of the Stimulated Raman Scattering Instability in Two-Dimensional Particle-In-Cell Simulations, Phys. Plasmas 17, 092704 (2010)

129. N. Naseri, D. Pesme, **W. Rozmus**, K. Popov, Channeling of relativistic laser pulses, surface waves and electron acceleration, Phys. Rev. Letters 108, 105001 (2012)

130. Xuan-Tao Su, Yuanyuan Qiu, L. Marquea-Curtis, M. Gupta, C. E. Capjack, **W. Rozmus**, A. Janowska-Wieczorek and Ying Y. Tsui, Label-free and noninvasive optical detection of the distribution of nanometer-size mitochondria in single cells, J. Biomedical Optics 16, 067003 (2011)

131. Xuan-Tao Su, S. E. Kirkwood, M. Gupta, L. Marquea-Curtis, Yuanyuan Qiu, A. Janowska-Wieczorek, **W. Rozmus** and Ying Y. Tsui, Microscope-Based Label Free Microfluidic Cytometry, Optics Express 19, 387 (2011)

132. I Silin, **RD Sydora**, IR Mann, K Sauer and RL Mace. "Nonlinear evolution of electromagnetic ion cyclotron waves" Phys. Plasmas 18 (2011), pp. 042108-042108-8.

133. RL Mace, **RD Sydora** and I Silin. "Effects of superthermal ring current ion tails on the electromagnetic ion cyclotron instability in multi-ion magnetospheric plasmas" J. Geophys. Res. 116 (May 2011): A05206.

134. I Silin, IR Mann, **RD Sydora**, D Summers and RL Mace. "Warm plasma effects on electromagnetic ion cyclotron wave MeV electron interactions in the magnetosphere" J. Geophys. Res. 116 (2011): A05215.

135. K Sauer and **RD Sydora**. "Whistler-Langmuir oscillitons and their relation to auroral hiss" Anal. Geoph. 29 (2011): 1739-1753.

136. I Silin and **RD Sydora**, Hybrid Fourier-Vlasov simulation in non-inertial reference frames, Comp. Phys. Comm., 182 (2011): p. 2508-2518.

137. K Sauer and **RD Sydora**. "Mode crossing effects as electron beam-plasma interaction and related phenomena" Plasma Phys. Control. Fusion , 54, 124045 (2012).

138. K Fujimoto and **RD Sydora**, Plasmoid-induced turbulence in collisionless magnetic reconnection, Phys. Rev. Lett., 109, 265004 (2012).

139. T Tacke, J Dreher and **RD Sydora**, Numerical magnetohydrodynamic simulations of expanding flux ropes: Influence of boundary driving, Phys. Plasmas, 20, 072104 (2013).

140. M.Ladrem, M.Chekerker, **F.C.Khanna** and A.E.Santana, Fragmentation Function in Thermofield Dynamics, Int.J.Mod.Physics A 28(2013)1350032

141. R.G.G. Amorim, M.C.B.Fernandes, **F.C.Khanna**, A.E.Santana and J.D.M.Vianna, Solutions for the Landau problem using Representations of the Galilei Group, Int.J.Mod.Phys.A 28(2013)1350013

142. Finite size effects on the phase transition in the three-dimensional Gross-Neveu model, **FC Khanna**, APC Malbouisson, JMC Malbouisson and AE Santana, EPL 97(2012)11002

143. Classical and quantum-mechanical state reconstruction, **FC Khanna**, PA Mello and M.Revzen, European J.Physics 33(2012)921-939.

144. Phase transition in the massive Gross-Neveu model in Toroidal topologies, **FC Khanna**, APC Malbouisson, JMC Malbouisson asnd AE Santana Phys.Rev.D85(2012)085105 (14 Pages)

145. **FC Khanna**, APC Malbouisson, JMC Malbouisson and AE Santana Quantum Fields in Toroidal topology, Annals of Physics (NY)328(2011)2634-2657.

146. J.Ramos-Medina, **M.de Montigny and FC Khanna**, On group theoretical approach to the Curl Operator, Int.J.Theoretical Phys.,Group Theory and non-linear optics 15(2011) 59-66.

147. S.C.Ulhoa, **FC Khanna** and AE Santana, Teleparallel formalism of Galilean Gravity, Russian J.Gravitation and Cosmology,!7(2011)242-251.

148. M.Chekerker,**FC Khanna** and AE Santana Thermofield Dynamics and e^{+}–e^{-} reactions, Int.J.Mod.Physics A 26 (2011) 2881-2897.

149. N.B. Lovett, C. Crosnier, M. PerarnauLlobet and **B. C. Sanders**, Differential Evolution for Many-Particle Adaptive Quantum Metrology, Physical Review Letters 110: 220501 (4 pp.), 28 May 2013.

150. M. Adcock, P. Hyer and **B. C. Sanders**, Gaussian quantum computation with oracledecision problems, Quantum Information Processing 12(4): 1759-1779, 1 April 2013.

151. R. H. Choi, B. Fortescue, G. Gour and **B. C. Sanders**, Entanglement sharing protocol via quantum error correcting codes, Physical Review A 87(3): 032319 (7 pp.), 15 March 2013.

152. S.H. Tan, Y. Y. Gao, H. de Guise and **B. C. Sanders**, SU(3) Quantum Interferometry with single-photon input pulses, Physical Review Letters 110(11): 113603 (5 pp.), 12 March 2013.

153. P. Xue and **B. C. Sanders**, Controlling and reversing the transition from classical diffusive to quantum ballistic transport in a quantum walk by driving the coin, Physical Review A 87(2): 022334 (7 pp.), 22 February 2013.

154. A. de la Lande, N. S. Babcock, J. Řezáč, **B. C. Sanders** and D. R. Salahub, Correction: Surface residues dynamically organize water bridges to enhance electron transfer between proteins (PNAS, vol 107, pg 11799, 2010), Proceedings of the National Academy of Sciences 110(28): 1136, 15 January 2013.

155. P. M. Leung and **B. C. Sanders**, Coherent control of microwave pulse storage in superconducting circuits, Physical Review Letters 109(25): 253603 (5 pp.), 18 December 2012.

156. J. S. Kim, G. Gour and **B. C. Sanders**, Limitations to sharing entanglement, Contemporary Physics 53(5): 417-432, 17 October 2012.

157. P. Xue, Z. Ficek and **B. C. Sanders**, Probing multipartite entanglement in a coupled Jaynes Cummings system, Physical Review A 86(4): 043826 (10 pp.), 16 October 2012.

158. S. Raeisi, N. Wiebe and **B. C. Sanders**, Quantum-circuit design for efficient simulations of manybody quantum dynamics, New Journal of Physics 14(10): 103017 (26 pp.), 9 October 2012.

159. B. Lavoie, P. M. Leung and **B. C. Sanders**, Low-loss surface modes and lossy hybrid modes in metamaterial waveguides, Photonics and Nanostructures – Fundamentals and Applications 10(4): 602 614, 14 September 2012.

160. **B. C. Sanders**, Review of entangled coherent states, Journal of Physics A: Mathematical and Theoretical 45(24): 244002 (22 pp.), 30 May 2012.

161. M. Siomau, A. A. Kamli, S. A. Moiseev and **B. C. Sanders**, Entanglement creation with negative index metamaterials, Physical Review A 85(5): 050303(R) (4 pp.), 15 May 2012.

162. A. de la Lande, N. S. Babcock, J. Řezáč, B. Lévy, **B. C. Sanders** and D. R. Salahub, Quantum effects in biological electron transfer, Physical Chemistry Chemical Physics 14(17): 5902 5918, 20 March 2012.

163. Y. J. Wang, **B. C. Sanders**, B.-M. Bai and X.-M. Wang, Enhanced feedback iterative decoding of sparse quantum codes, IEEE Transactions on Information Theory 58(2): 1231 1241, 6 February 2012.

164. P. Xue and **B. C. Sanders**, Two quantum walkers sharing coins, Physical Review A 85(2): 022307 (8 pp.), 6 February 2012.

165. A. Hentschel and **B. C. Sanders**, An efficient algorithm for optimizing adaptive quantum metrology processes, Physical Review Letters 107(23): 233601 (4 pp.), 30 November 2011.

166. N. Wiebe, D. W. Berry, P. Hyer and **B. C. Sanders**, Simulating quantum dynamics on a quantum computer, Journal of Physics A: Mathematical and General 44(44): 445308 (20 pp.), 18 October 2011.

167. P. M. Anisimov, J. P. Dowling and **B. C. Sanders**, Objectively discerning Autler-Townes splitting from electromagnetically induced transparency, Physical Review Letters 107(16): 163604 (4 pp.), 12 October 2011.

168. B. Toloui, G. Gour and **B. C. Sanders**, Constructing monotones for quantum phase references in totally dephasing channels, Physical Review A 84(2): 022322 (8 pp.), 17 August 2011.

169. J. S. Kim and **B. C. Sanders**, Unified entropy, entanglement measures and monogamy of multiparty entanglement, Journal of Physics A: Mathematical and Theoretical 44(29): 295303 (14 pp.), 20 June 2011.

170. A. de la Lande, J. Řezáč, B. Lévy, **B. C. Sanders** and D. R. Salahub, Transmission coefficients for chemical reactions with multiple states: Role of quantum decoherence, Journal of the American Chemical Society 133(11): 3883 3894, 23 March 2011.

171. A. Hentschel and **B. C. Sanders**, Ordered measurements of permutation-invariant qubit strings, Journal of Physics A: Mathematical and Theoretical 44(11): 115301 (16 pp.), 18 February 2011.

172. A. Scherer, **B. C. Sanders** and W. Tittel, Long-distance practical quantum key distribution by entanglement swapping, Optics Express 19(4): 3004 3018, 1 February 2011.

173. S. Lee, J. S. Kim and **B. C. Sanders**, Distribution and dynamics of entanglement in highdimensional quantum systems using convexroof extended negativity, Physics Letters A 375(3): 411 414, 17 January 2011.

174. D. Markham and **B. C. Sanders**, Erratum: Graph states for quantum secret sharing [Phys. Rev. A 78, 042309 (2008)], Physical Review A 83(1): 019901(E) (1 p.), 11 January 2011.

175. S. Rahimi-Keshari, A. Scherer, A. Mann, A. T. Rezakhani, A. I. Lvovsky and **B. C. Sanders**, Quantum process tomography with coherent states, New Journal of Physics 13(1): 013006 (17 pp.), 11 January 2011, arXiv.org:1009.3307. Selected for New Journal of Physics Highlights of 2011 Collection.

176. A. Kamli, S. A. Moiseev and **B. C. Sanders**, Quantum informatics with plasmonic metamaterials, International Journal of Quantum Information 9(supplementary issue 1): 263 279, 1 January 2011.

177. **A. Czarnecki**, "Recent developments in higher order precision calculations at lower energies," PoS LL 2012, 006 (2012).

178. **A. Czarnecki**, M. Kamionkowski, S. K. Lee and K. Melnikov, "Charged Particle Decay at Finite Temperature," Phys. Rev. D 85, 025018 (2012)

179. N. Blinov and **A. Czarnecki**, "Binding energy of the positronium negative ion via dimensional scaling," Phys. Rev. A 85, 012522 (2012)

180. Y. Liang and **A. Czarnecki**, "Photon-photon scattering: A Tutorial," Can. J. Phys. 90, 11 (2012)

181. **A. Czarnecki**, X. Garcia i Tormo and W. J. Marciano, "Muon decay in orbit spectra for $\mu - e$ conversion experiments," Hyperfine Interact. 210, 19 (2012)

182. X. Garcia i Tormo, D. Bryman, **A. Czarnecki** and M. Dowling, "Bounds on majoron emission from muon to electron conversion experiments," Phys. Rev. D 84, 113010 (2011)

183. **A. Czarnecki**, X. Garcia i Tormo and W. J. Marciano, "Muon decay in orbit: spectrum of high-energy electrons," Phys. Rev. D 84, 013006 (2011)

184. **A.. Penin** and J.H. Piclum *Threshold production of unstable top*, JHEP, 1201, (2012) 034

185. **A.A. Penin** and G. Ryan *Two-loop electroweak corrections to high energy large-angle Bhabha scattering*, JHEP, 1111,(2011) 081,

186. J.H. Kuhn, F. Metzler, **A.A. Penin**, and S. Uccirati, *Next-to-Next-to-Leading Electroweak Logarithms for W-Pair Production at LHC*, JHEP, 1106, (2011) 143

187. **A.A. Penin** *Measuring Vacuum Polarization with Josephson Junctions*, Phys.Rev.Lett., 104, (2010) 097003

188. S. M. Ibrahim Al-Rafia, M. R. Momeni, R. McDonald, M. J. Ferguson, **A. Brown** and E. Rivard, 2013, Stable Complexes of Parent Digermene: an Inorganic Analogue of Ethylene, Organometallics, accepted dx.doi.org/10.1021/om400361n [Special Issue: Applications of Electrophilic Main Group Organo- metallic Molecules]

189. S. M. Ibrahim Al-Rafia, M. R. Momeni, R. McDonald, M. J. Ferguson, **A. Brown** and E. Rivard, 2013, Controlled Growth of Dichlorogermanium Oligomers from Lewis Basic Hosts, accepted Angew. Chemie. Int. Ed. 52 6390-6395 (VIP Article).

190. M. Gedik and **A. Brown**, 2013, Computational Study of the Excited State Properties of Modified RNA Nucleobases, J. Photochem. And Photobiol. A: Chemistry, 259 25-32.

191. E. Pradhan, J.-L. Carreon-Macedo, J.E. Cuervo, M. Schroeder, and **A. Brown**, 2013, Ab initio potential energy and dipole moment surfaces for CS2: Determination of Molecular Vibrational Energies, J. Phys. Chem. A, accepted dx.doi.org/10.1021/jp309651r [Joel M. Bowman Festschrift]

192. E.K. Campbell, A.B. Alekseyev, G.G. Balint-Kurti, M. Brouard, **A. Brown**, R.J. Buenker, A.J. Johnsen, D.B. Kokh, S. Lucas, , and B. Winter, 2012, The vibrationally mediated photodissociation of Cl2, J. Chem. Phys. 136 0164311 (16 pages).

193. **A. Brown** and R.E. Wasylishen, 2012, Nuclear quadrupole coupling constants for N2O: Experiment and Theory, J. Phys. Chem. A 116, 9769-9776.

194. R.R. Zaari and **A. Brown**, 2012, Effect of Laser Pulse Shaping Parameters on the Fidelity of Quantum Logic Gates, J. Chem. Phys. 137, 104306 (12 pages).

195. E.K. Campbell, A.B. Alekseyev, G.G. Balint-Kurti, M. Brouard, **A. Brown**, R.J. Buenker, R. Cireasa, A.J. Gilchrist, A.J. Johnsen, D.B. Kokh, S. Lucas, G.A.D. Ritchie, T.R. Sharples, and B. Winter, 2012 Electronic polarization effects in the photodissociation of Cl2, J. Chem. Phys. 136 0164311 (16 pages).

196. A.J. Johnsen, A.B. Alekseyev, G.G. Balint Kurti, M. Brouard, **A. Brown**, R.J. Buenker, E.K. Campbell, and D.B. Kokh, 2012, A complete quantum mechanical study of chlorine dissociation, J. Chem. Phys. 136 0164310 (15 pages).

197. L. Liu, K. Michelsen, E.N. Kitova, P.D. Schnier, **A. Brown**, and J. S. Klassen, 2012, Dissociation of a Protein-Fatty Acid Complex in the Gas Phase. Kinetic Isotope Effects Suggest a Late Transition State, J. Am. Chem. Soc. 134, 5931-5937.

198. **A. Brown**, T.Y. Ngai, M.A. Barnes, J.A. Key, and C.W. Cairo, 2012, Substituted benzoxadiazoles as fluorogenic probes: A computational study of absorption and fluorescence, J. Phys. Chem. A 116 46-54.

199. R.R. Zaari and **A. Brown**, 2011, Effect of diatomic molecular properties on binary laser pulse optimizations of quantum gate operations, J. Chem. Phys., 135 044317 (7 pages).

200. S.Y.Y. Wong, D. Benoit, M. Lewernz, **A. Brown** and P.-N. Roy, 2011, Determination of Molecular Vibrational Energies using the ab initio Semiclassical Initial Value Representation: Application to formaldehyde, J. Chem. Phys., 134 094110 (10 pages).

201. Sow, C. S.; Tomkins, J.; **Hanna, G.** "Computational study of the one- and two-dimensional infrared spectra of a proton transfer mode in a hydrogen-bonded complex dissolved in a polar nanocluster" ChemPhysChem, in press.

202. **Hanna, G.**; Kapral R. Quantum-Classical Liouville Dynamics of Condensed Phase Quantum Processes in ReactionRateConstantComputations: TheoriesandApplications,editedbyK. Han and T. Chu (The Royal Society of Chemistry Theoreticaland ComputationalChemistrySeries No. 6, 2013), in press.

203. Martinez, F; Rekik, N.; **Hanna, G.** "Simulation of nonlinear optical signals via approximate solutions of the quantum-classical Liouville equation: Application to the pump-probe spectroscopy of a condensed phase electron transfer reaction" Chemical Physics Letters, 2013, 573: 77-83.

204. Rekik, N.; Hsieh C-Y; Freedman, H.; **Hanna, G.** "A mixed quantum-classical Liouville study of the population dynamics in a model photo-induced condensed phase electron transfer reaction" Journal of Chemical Physics, 2013, 138: 144106(1)-144106(12).

205. Rekik, N.; **Hanna, G.** "Explaining the Structure of the OH Stretching Band in the IR Spectra of Strongly Hydrogen-Bonded Dimers of Phosphinic Acid and their Deuterated Analogs in the Gas Phase: A Computational Study" Journal of Physical Chemistry A, 2012, 116: 4495-4509.

206. Galib, M.; **Hanna, G.** "Mechanistic Insights into the Dissociation and Decomposition of Carbonic Acid in Water via the Hydroxide Route: An ab-initio Metadynamics Study" Journal of Physical Chemistry B, 2011, 115: 15024-15035.

207. **Hanna, G.**; Geva, E. "Signature of Nonadiabatic Transitions on the Pump-Probe Infrared Spectra of a Hydrogen-Bonded Complex Dissolved in a Polar Solvent: A Computational Study" Journal of Physical Chemistry B, 2011, 115: 51915200.

208. **Hanna, G.**; Geva, E. "Computational study of the signature of hydrogen-bond strength on the infrared spectra of a hydrogen-bonded complex dissolved in a polar liquid" Chemical Physics, 2010, 370: 201-207.

209. Tao Zeng, Dmitri G. Fedorov, and **Mariusz Klobukowski** "Performance of dynamically weighted multiconfiguration self-consistent field and spin-orbit coupling calculations of diatomic molecules of Group 14 elements" Journal of Chemical Physics, 134 (2011) 024108-1 024108-11.

210. Jocelyne Shim, **Mariusz Klobukowski**, Maria Barysz, Jerzy Leszczynski "Calibration and applications of ΔMP2 method for calculating core electron binding energies" Physical Chemistry Chemical Physics, 13 (2011) 5703-5711.

211. Tao Zeng, Dmitri G. Fedorov, Michael W. Schmidt, and **Mariusz Klobukowskii** "Two-component natural spinors from two-step spin-orbit coupled wave functions" Journal of Chemical Physics, 134 (2011) 214107-1 214107-9.

212. Evan Kelly, **Jack Tuszynski**, and **Mariusz Klobukowski** "QM and QM/MD Simulations of the Vinca Alkaloids Docked to Tubulin" Journal of Molecular Graphics and Modeling, 30 (2011) 54 66.

213. Tao Zeng, Dmitri G. Fedorov, Michael W. Schmidt, and **Mariusz Klobukowski** "Effects of spin-orbit coupling on covalent bonding and the Jahn-Teller effect are revealed with the natural language of spinors" Journal of Chemical Theory and Computation, 7 (2011) 2864 2875.

214. Hirotoshi Mori, Tao Zeng, **Mariusz Klobukowski** "Assessment of Chemical Core Potentials for the Computation on Enthalpies of Formation of Transition-metal Complexes" Chemical Physics Letters, 521 (2012) 150 156.

215. Tao Zeng and **Mariusz Klobukowski** "Guide to Programs for Non-relativistic Quantum Chemistry Calculations", invited chapter in Handbook of Computational Chemistry, Chapter 17, pp. 612 630. Springer 2012

216. Tao Zeng and **Mariusz Klobukowski** "Model core potentials in the first decade of the XXI century", invited chapter in Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends, Springer 2011

217. Maria Barysz, **Mariusz Klobukowski**, Jerzy Leszczynski "Relativistic study of tautomerism and core electron binding energies of thio- and seleno-cytosine" Structural Chemistry, 23 (2012) 1293 1299.

218. Tao Zeng, Dmitri G. Fedorov, Michael W. Schmidt, and **Mariusz Klobukowski** Natural Spinors Reveal How the Spin-Orbit Coupling Affects the Jahn-Teller Distortions in the Hexafluorotungstate(V) Anion Journal of Chemical Theory and Computation, 8 (2012) 3061 3071.

219. Amelia Fitzsimmons and **Mariusz Klobukowski** "Structure and Stability of Organic Molecules Containing Heavy Rare Gas Atoms" Theoretical Chemistry Accounts, 132 (2013) 1314

220. T. Zeng, G. Guillon, J. T. Cantin, and **P.-N. Roy**, "Probing a molecular superfluid with an asymmetric top impurity", http://dx.doi.org/10.1021/jz401188j.

221. L. Wang, D. Xie, R. J. Le Roy, and **P.-N. Roy**, A new six-dimensional potential energy surface for H2N2O and its adiabatic-hindered-rotor treatment, accepted

222. S. Constable, M. Schmidt, C. Ing, T. Zeng, and **P.-N. Roy**, "Langevin Equation Path Integral Ground State", http://dx.doi.org/10.1021/jp4015178.

223. Y. Tritzant-Martinez,T. Zeng, A. Broom, E. Meiering, R. J. Le Roy, and **P.-N. Roy** On the analytical representation of free energy profiles with a Morse/Long-Range model: application to the water dimer, J. Chem. Phys. 138, 234103 (2013); http://dx.doi.org/10.1063/1.4810006

224. Grgoire Guillon, Tao Zeng, and **Pierre-Nicholas Roy**, On the origin and convergence of a post-quantization constrained propagator for path integral simulations of rigid bodies, J. Chem. Phys. 138, 184101 (2013); http://dx.doi.org/10.1063/1.4803118

225. T. Zeng, H. Li, and **P.-N. Roy**, Simulating asymmetric top impurities in superfluid clusters: a para-water dopant in para-hydrogen, J. Phys. Chem. Lett. 4, 18 (2013); DOI: 10.1021/jz3017705

226. L. Wang, D. Xie, R. J. Le Roy, and **P.-N. Roy**, A new four-dimensional ab initio potential energy surface for N2O-He and vibrational band origin shifts for the N2O-HeN clusters with N =1 40, J. Chem. Phys. 137, 104311 (2012); http://dx.doi.org/10.1063/1.4749248 (7 pages)

227. S. M. Islam, and **P.-N. Roy**, "Performance of the SCC-DFTB model for the description of five-membered ring carbohydrate conformations: comparison to forcefields, high-level electronic structure methods, and experiment", J. Chem. Theory Comput., 2012, 8 (7), pp 24122423 DOI: 10.1021/ct200789w

228. P. L. Raston, W. Jger, H. Li, R. J. Le Roy, and **P.-N. Roy** Rotational Study of Carbon Monoxide Solvated with para-Hydrogen Molecules: Evidence for Superfluid Molecular Hydrogen, Phys. Rev. Lett. 108, 253402 (2012) URL: http://link.aps.org/doi/10.1103/PhysRevLett.108.253402 DOI: 10.1103/PhysRevLett.108.253402

229. C. Ing, J. Yang, K. Hinsen, T. Zeng, H. Li, and **P.-N. Roy**, A path-integral Langevin equation treatment of low-temperature doped helium clusters, J. Chem. Phys. 136, 224309 (2012). URL: http://link.aip.org/link/?JCP/136/224309 DOI: 10.1063/1.4726507

230. Ultrasound Imaging of Long Bone Fractures and Healing with the Split-Step Fourier Imaging Method, H Li, LH Le, **MD Sacchii**, EHM Lou Ultrasound in Medicine & Biology 39 (8), 1482-1490, (2013)

231. Vector reconstruction of multicomponent seismic data, A Stanton, **MD Sacchi** GEOPHYSICS 78 (4), (2013)

232. A fast reduced-rank interpolation method for prestack seismic volumes, that depend on four spatial dimensions J Gao, **MD Sacchi**, X Chen Geophysics 78 (1), V21-V30, (2013)

233. Multidimensional de-aliased Cadzow reconstruction of seismic records, M Naghizadeh, **M Sacchi** Geophysics 78 (1), (2013)

234. A compressive sensing framework for seismic source parameter estimation I Vera Rodriguez, **M Sacchi**, YJ Gu Geophysical Journal International 191 (3), 1226-1236, (2012)

235. Bayesian linearized seismic inversion with locally varying spatial anisotropy, EL Bongajum, J Boisvert, MD Sacchi Journal of Applied Geophysics, (2012)

236. A tensor higher-order singular value decomposition for prestack seismic data noise reduction and interpolation, N Kreimer, **MD Sacchi** Geophysics 77 (3), V113-V1227, (2012)

237. Edge-preserving seismic imaging using the total variation method, AY Anagaw, **MD Sacchi** Journal of Geophysics and Engineering 9 (2), 138, (2012)

238. Simultaneous recovery of origin time, hypocentre location and seismic moment tensor using sparse representation theory, IV Rodriguez, **M Sacchi**, YJ Gu Geophysical Journal International 188 (3), 1188-1202, (2012)

239. Multicomponent f-x seismic random noise attenuation via vector autoregressive operators, M Naghizadeh, M Sacchi Geophysics 77 (2), V91-V99, (2012)

240. Microseismic data denoising using a 3C group sparsity constrained time-frequency transform, I Vera Rodriguez, D Bonar, **M Sacchi** Geophysics 77 (2), V21-V29, (2012)

241. Denoising seismic data using the nonlocal means algorithm, D Bonar, **M Sacchi** Geophysics 77 (1), A5-A8, (2012)

242. Shear wave reflectivity imaging of the Nazca-South America subduction zone: Stagnant slab in the mantle transition zone? S Contenti, YJ Gu, A Ökeler, **MD Sacchi** Geophysical Research Letters 39 (2), (2012)

243. Resolution of Seismic-Moment Tensor Inversions from a Single Array of Receivers, IV Rodriguez, YJ Gu, **MD Sacchi** Bulletin of the Seismological Society of America 101 (6), 2634-2642, (2011)

244. High-resolution three-term AVO inversion by means of a Trivariate Cauchy probability distribution, W Alemie, **MD Sacchi** Geophysics 76 (3), R43-R55, (2011)

245. Simultaneous seismic data denoising and reconstruction via multichannel singular spectrum analysis, V Oropeza, **M Sacchi** Geophysics 76 (3), V25-V32, (2011)

246. Numerical analysis of wave-induced fluid flow effects on seismic data: Application to monitoring of CO2 storage at the Sleipner field, J Rubino, DR Velis, **MD Sacchi** Journal of Geophysical Research: Solid Earth (19782012) 116 (B3), (2011)

247. Probing the Effect of Side-Chain Length on the Aggregation of a Model Asphaltene Using Molecular Dynamics Simulations, C Jian, T Tang, **S Bhattacharjee** Energy & Fuels 27 (4), 2057-2067 (2013)

248. Electric field assisted cross flow micellar enhanced ultrafiltration for removal of naphthenic acid, B Venkataganesh, A Maiti, **S Bhattacharjee**, S De Separation and Purification Technology 98, 36-45, (2012)

249. High-power electrokinetic energy conversion in a glass microchannel array, A Mansouri, **S Bhattacharjee**, L Kostiuk Lab Chip 12 (20), 4033-4036, (2012)

250. Study on the use of dielectrophoresis and electrothermal forces to produce on-chip micromixers and microconcentrators, NSK Gunda, **S Bhattacharjee**, SK Mitra Biomicrofluidics 6, 034118, (2012)

251. Characterization of Boiler Blowdown Water from Steam-Assisted Gravity Drainage and SilicaOrganic Coprecipitation during Acidification and Ultrafiltration, A Maiti, M Sadrezadeh, S Guha Thakurta, DJ Pernitsky, **S Bhattacharjee** Energy & Fuels 26 (9), 5604-5611, (2012)

252. Sherwood number in flow through parallel porous plates (Microchannel) due to pressure and electroosmotic flow, N Vennela, S Mondal, S De, **S Bhattacharjee** AIChE Journal 58 (6), 1693-1703, (2012)

253. Probing Structure – Nanoaggregation Relations of Polyaromatic Surfactants: A Molecular Dynamics Simulation and Dynamic Light Scattering Study, RB Teklebrhan, L Ge, **S Bhattacharjee**, Z Xu, J Sj oblom The Journal of Physical Chemistry B 116 (20), 5907-5918,(2012)

254. Parametric energy conversion of thermoacoustic vibrations, C Guthy, CW Van Neste, S Mitra, **S Bhattacharjee**, T Thundat Applied Physics Letters 100 (20), 203902-203902-4, (2012)

255. Particle transport in patterned cylindrical microchannels, R Chatterjee, **S Bhattacharjee**, SK Mitra Microfluidics and nanofluidics 12 (1-4), 41-51, (2012)

256. A systematic evaluation of the role of crystalline order in nanoporous materials on DNA separation, N Nazemifard, L Wang, W Ye, **S Bhattacharjee**, JH Masliyah, DJ Harrison Lab on a Chip 12 (1), 146-152, (2012)

257. Sherwood number in porous microtube due to combined pressure and electroosmotically driven flow, N Vennela, **S Bhattacharjee**, S De Chemical Engineering Science 66 (24), 6515-6524, (2011)

258. Influence of electrostatic and chemical heterogeneity on the electric-field-induced destabilization of thin liquid films, A Atta, DG Crawford, CR Koch, **S Bhattacharjee** Langmuir 27 (20), 12472-12485, (2011)

259. Integration of rotational algorithms into dissipative particle dynamics: modeling polyaromatic hydrocarbons on the meso-scale, SF Zhang, JB Xu, H Wen, **S Bhattacharjee** Molecular Physics 109 (15), 1873-1888, (2011)

260. Particle deposition onto janus and patchy spherical collectors, R Chatterjee, SK Mitra, **S Bhattacharjee** Langmuir 27 (14), 8787-8797, (2011)

261. Structure – activity relationships of an antimicrobial peptide plantaricin S from two-peptide class IIb bacteriocins, W Soliman, L Wang, **S Bhattacharjee**, K Kaur Journal of medicinal chemistry 54 (7), 2399-2408

262. Flux decline during cross flow membrane filtration of electrolytic solution in presence of charged nanocolloids: A simple electrokinetic model, S De, **S Bhattacharjee** Journal of colloid and interface science 353 (2), 530-536