Nanoscale Systems MMTA • ISSN: 2299-3290
Editorial • DOI: 10.2478/nsmmt-2013-0001 • NanoMMTA • Vol. 2 • 2013 • 1-9

Multidisciplinary approaches in theory, applications and modeling of nanoscale systems

Abstract

This editorial provides an overview of both fundamental and applied research areas covered by the journal of *Nanoscale Systems: Mathematical Modeling, Theory and Applications* (NanoMMTA), as well as of articles published in the journal inaugural volume. The unique feature of NanoMMTA is its focus on the interface between the study, development, and application of systems at the nanoscale with theoretical methods and experimental techniques on the one hand and mathematical, statistical, and computational tools on the other. NanoMMTA is the first international, interdisciplinary, peer-reviewed journal focusing specifically on this interface. This emerging multidisciplinary field at the interface of mathematical modeling, nanoscience and nanotechnology includes applications and advancements of these tools in all of the disciplines facing the challenges associated with the nanoscale systems.

Keywords

Systems at the nanoscale • Physics and chemistry • Biology and life sciences • Materials science • Medicine and engineering • Mathematical, statistical and computational sciences • Cross-disciplinary research collaboration

PACS: 61.46.-w, 65.80.-g, 62.25.-g, 73.63.-b, 62.23.-c, 64.70.Nd, 75.75.-c, 36.40.-c, 63.22m, 68.65.-k, 74.78.-w, 78.67.-n, 81.07.-b, 81.16.Rf, 87.85.J-, 82.35.Pq, 85.35.-p, 85.85.+j, 87.10.-e, 87.85.Qr, 87.85.Rs, 87.85.Tu, 88.30.rh, 81.16.-c, 81.40.-z

MSC: 82D, 97M, 81T, 35Q, 65D, 46N, 20G, 58D, 68Q, 81-XX, 94A

© **Versita sp. z o.o.**

Roderick V. N. Melnik[1]*

1 *M²NeT Laboratory, Faculty of Science, Wilfrid Laurier University, 75 University Avenue West, Waterloo, ON, Canada N2L 3C5*

Received 21 December 2012
Accepted 16 January 2013

1. Systems at the Nanoscale are Ubiquitous in Nature and a Man-Made World

Systems at the nanoscale are ubiquitous in a wide range of technological innovations, as well as in nature. Examples include low dimensional semiconductor nanostructures such as quantum wires and quantum dots, carbon nanostructures such as graphene and nanotubes, and a diverse variety of biological nanostructures such as those obtained from biomolecules, to name just a few. Our study of such systems is of both fundamental and applied importance. Moreover, such systems are central to our better understanding and ultimate rational design of larger systems in which nanoscale systems are integrated. By now, it has become evident that in the study, development, and application of systems at the nanoscale, along with experimental techniques, mathematical, statistical, and computational tools emerge as absolutely decisive for our overall success. This emerging multidisciplinary field at the interface of mathematical modeling, nanoscience and nanotechnology includes applications and advancements of these tools in all of the disciplines facing the challenges associated with the nanoscale systems. This includes, but not limited to: physics, chemistry, biology, materials science, medicine, and engineering.

* *E-mail: rmelnik@wlu.ca*

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

NanoMMTA is the first international, interdisciplinary, peer-reviewed journal focusing specifically on this interface. It serves its diverse readership by covering important advances in all aspects of nanoscale systems that are being achieved with mathematical, statistical and computational tools, as well as advances in the development of mathematical theory and applications pertinent to such systems. The peer-review system for this journal, together with the outstanding scientists of the editorial board, ensures that quality is maintained throughout. It is a unique publication medium, devoted to and promoting a multidisciplinary approach in meeting new challenges faced by theory, applications and modeling of nanoscale systems.

As the continuously growing range of areas in science, engineering and other human endeavors are inevitably becoming increasingly quantitative, the progress in all such areas will be more and more dependent on the successful development of advanced mathematical, statistical and modeling methodologies and techniques [1, 2]. The field of nanoscience and nanotechnology is one of the most prominent examples of this tendency.

Recognizing the importance and continuity of this tendency in the progress of a growing number of areas, the NanoMMTA journal provides a forum for studying

- nanoscale systems in physics and chemistry;
- nanoscale systems in life sciences and medicine;
- nanoscale systems in materials science and engineering;
- nanoscale systems in environmental and sustainability sciences;
- nanoscale systems in advanced technologies;
- nanoscale systems in non-traditional and emerging areas;
- coupled phenomena and processes in nanoscale systems;
- integration of nanoscale systems into larger structures with interacting components;
- fundamentals and applications of dynamics at the nanoscale;
- mathematical foundations, analysis and modeling of nanoscale systems.

In the context of nanoscience and nanotechnology, boundaries between different disciplines (e.g., physics and chemistry, biology and physics, mathematics and computational science, chemistry and biology, etc) become increasingly intangible, opening opportunities for a larger cross-disciplinary research collaboration and necessitating the development of new multidiscilinary approaches to new challenging problems arising in this field. In what follows we briefly highlight some of these problems and areas covered by the above list, without prioritizing them.

1.1. Nanobiomedicine, bionanotechnologies, and nanoscale systems in life sciences

This includes biological and biomimetic nanomaterials (e.g., as therapeutics), as well as nanodevices for medical and biological applications. Examples are nanobiomembranes, nanopharmaceuticals, nanobiomarkers, nanobiolabels, biocapsules, nanobiosensors, nanobiomotors and their applications, as well as relevant technologies, instrumentation techniques for nanobioscience, nanoscale cellular and tissue engineering, etc. An interesting example also includes the use of quantum dots to visualize cellular processes and protein-protein interactions. We are interested here in developing and applying tools of mathematical, computational and statistical sciences to the above examples as well as to

- carbon nanotubes in biological and biomedical applications;
- the delivery, detection, and labelling of nanoparticles for targeted drug release, drug and gene delivery in biological systems, and, more generally the clinical application of nanoscience materials, tools, and methods;
- nanodiagnostics and disease control, nanobioimaging technologies;
- nucleic acids (DNA and RNA) nanotechnologies, nanoscale proteomics and genomics;

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

- nanotoxicology (e.g., of drug delivery carriers), nanoscale physiology and pathology;
- bionanoelectromechanical systems, lab-on-a-chip technologies, and their applications;
- biological processes and phenomena at the nanoscale;
- other areas of nanobiomedicine and nanobiotechnologies.

1.2. Nanoscale materials, their properties, characterization, and applications

Nanomaterials are currently used in a wide variety of applications and the list continues to rapidly grow, from construction, design and architecture to water quality, enhanced catalysis and oil recovery. Such nanomaterials include also bioplymers, nanocomposites, nanoporous materials, magnetic/spintronic nanomaterials, as well as hybrid nanomaterials such as inorganic-organic, inorganic-inorganic and organic-organic. For example, biopolymeric nanocrystalline cellulose' current and potential applications include cosmetics and anti-bacterial coating, pulp and paper products, automotive and aerospace industries. Depending on the specific application area, we are interested in various properties of nanomaterials such as electrical, optical, optoelectronic, magnetic, chemical, thermal, mechanical and other physical properties (size-dependent properties, as well as property-function relationships). The nanoscale systems of interest in this context include both soft and condensed matter nanomaterials such as nanotubes and polymeric capsules, nanostructured films and nanogels, core-shell nanosystems and living systems at the nanoscale. Nanomechanics of materials and biomaterials also becomes an important direction in the field. An example includes nanomechanics of biological tissues, e.g. bones. The nanomechanical spatial heterogeneity of bone stiffness is essential to account for in mathematical models. It is now known that the results accounting for this predict markedly different biomechanical properties compared with a uniform material [3]. Further insight, that can be obtained with mathematical modeling, may help in designing new biologically inspired materials technologies.

Advanced manufacturing nanomaterials-based technologies lead to further progress in such areas as nanomachining, nanorobotics, nanotribology, nanofluidics, molecular nanoscience and molecular electronics. Information processing, optical communications, quantum cryptography, packaging and nanointegration are all beneficiaries of this development, as well as the entire field of design of devices and device components based on nanomaterials.

The measurement of properties of nanomaterials and the development of experimental techniques to characterize them are difficult and important tasks. They are increasingly often supplemented by mathematical and computer modeling, allowing better understanding and prediction of properties of materials at the nanoscale.

1.3. Nanostructures, nanodevices and their integration

Nanostructures of interest include quantum dots, quantum wires, quantum wells, superlattices, nanoscale thin films, nanorods, nanotubes, nanostructure arrays, quantum dot molecules, molecular wires, fullerenes, nanoclusters, nanocrystals, nanoparticles, nanocapsules, nanofibers, nanocomposites and nanocomposite structures, as well as synthetic and natural nanocontainers, nanoreactors, nanocarriers of functional compounds. We are interested in properties and functions of these nanostructures and in devices with such nanostructure components. The latter includes semiconductor devices, nanoelectronic devices and circuits, electronic, optoelectronic, photonic and spintronic devices, nanoelectronic circuits, integrated multifunctional nanosystems, nanodevice integration and applications. Along with photonic devices, nanophotonics applications include problems in plasmonics and metamaterials, light-matter interaction and optical manipulation techniques. In sensing and actuating for nanoscale applications we are interested in nanosensors and monitoring nanodevices, including physical and mechanical sensing, chemical and biological detection and measurements, etc.

Interest is growing in the design and analysis of new complex nanostructures such as arrays of quantum dots and arrays of nanotubes [4]. This also includes graphene nanostructures such as graphene quantum dots and their arrays [5, 6]. The geometrical considerations are proven to be important in determining quantum mechanical and electronic properties. In [5], it was shown that the wavefunction of small molecular graphene structures can be different from those of larger nanoscale counterparts, while the distribution of the highest occupied molecular orbital is strongly affected by the geometric shape.

An increasing interest to graphene in the context of nanoelectronic devices and for other applications is due to the versatility of graphene-based devices, which goes beyond conventional transistor circuits and includes flexible

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

and transparent electronics, optoelectronics, sensors, electromechanical systems, and energy technologies [7]. Many challenges remain in studying properties of this material and especially graphene-based nanosystems and devices.

1.4. Processing methods at the nanoscale, synthesis, nanofabrication, self-assembly

Nanoscale manufacturing, materials synthesis techniques and materials characterization rely not only on advanced experimental techniques, but also increasingly on mathematical and computational tools. Nanofabrication is essentially the exploitation and control of self-organization phenomena for patterning where mathematical models can contribute substantially. The materials synthesis requires the fabrication and growth of materials with nanoscale precision and control. Similar to other processing methods, this growth can be modeled mathematically. Control over the morphology of surfaces on nanoscale becomes increasingly important in all modern science and engineering, from physics and chemistry to materials and life sciences. It is known, for example, that shape and form are decisive parameters in the nanoscale self-assembly [8]. Of special interest is mathematical modeling and foundations of self- and directed-assembly of nanostructures, as well as novel processing techniques in nanolithography and nanopatterning, nanocatalysis, and others.

1.5. Coupled and transport phenomena at the nanoscale, mathematical models

One of the standard examples of coupled systems at the nanoscale is provided by nanoelectromechanical systems (NEMS). Coupled systems are common place in nanoscience and nanotechnology [9–11]. Other typical examples where coupled (e.g., multiphysics) problems arise naturally in this field include: studies of nanothermoelectrics, nanocomposites, nanomagnetics, nanoscale radiation, and thermoelectric phenomena on the nanoscale, to name just a few.

In a number of applications we need to go beyond spatial complexity, because many such coupled problems need to be considered in a dynamic setting. Examples of this situation could be provided by nanoscale systems involving multiphase flows, bio/chemical reactions, spin excitations and dynamics of magnetic vortices and domain walls, spin waves and their optical applications. In photonics, ultrafast nonlinear pulse propagation in nano materials and structures is of special interest. Other areas of nanoscience and nanotechnology, such as semiconducting and magnetic nanostructures, optoelectronics and quantum computing, spintronics and information processing in nanosystems, all provide a multitude of examples of coupled dynamic problems. Continuing attempts to extend time scales in atomistic simulations lead to new development in mathematical and computational techniques. In [12], a new hybrid deterministic-stochastic approach, based on a combination of molecular dynamics (MD) and Monte Carlo (MC) simulations, has been proposed and demonstrated on an example of modeling source-controlled plasticity and deformation behavior in Au nanostructures. Recall also that RNA and DNA nanotechnologies rely essentially on studies of biological (biomolecular) nanostructures where new coarse-grained methodologies need to be developed [13]. New computational methodologies are also needed for studying dynamic biomolecule interactions at the nanoscale such as nanoscale protein-protein interactions, as well as protein organization and biochemical events at the nanoscale in living cell membranes [14]. Furthermore, in DNA and RNA nanotechnologies, nucleic acids represent important building blocks for the programmable construction of nanoscale systems that have an increasing range of applications in life and materials sciences. For example, based on the analogy with topological architectures of DNA molecules that condense and relax during cellular events, the authors of [15] demonstrate how complex and reconfigurable synthetic topological nanostructures can be engineered. They argue that their DNA fold-and-cut strategy may be used to create and reconfigure programmable topological nanostructures that are unprecedented in molecular engineering.

This is the area where, due to time-consuming and cost-intensive experimental validation of designed nanostructures the role of predictive physical-based mathematical models of nanostructures in the design process will be increasing drastically. Such mathematical models can significantly increase the number and variety of synthetic nanostructures designed using nucleic acids [16].

In all the above areas, the development of mathematical modeling and computational techniques becomes increasingly important. Moreover, many problems we have to deal with in this field requires multiscale approaches which are application driven. Take self-assembly as an example. Self-assembled nanostructures and devices have often to be studied across different scales (e.g., from nanoscale to mesoscale). Top-down and bottom-up approaches, applied in a combination, will also inevitably lead to scale coupling. Many problems in the field require such coupling (e.g., atomistic-to-continuum coupling), necessitating the development of novel mathematical and computational methodologies to study corresponding phenomena, processes and systems. New approaches are also required for analyzing and solving nonlinear mathematical models for quantum mechanics (e.g., Schrödinger and Schrödinger-Poisson systems).

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

The NanoMMTA journal welcomes contributions in both the mathematical and numerical analysis of such models and associated problems. Mathematical aspects of quantum models (including quantum theories in cosmology and life sciences), quantum algebra and quantum groups, quantum paradoxes, mathematics for quantum information processing and quantum computation, quantum algorithms and foundations are all in the scope of the journal.

Interesting recent developments in the study of complex classical systems via their quantum counterparts have been reported in [17]. It was argued that for both deterministic and stochastic mathematical models of classical systems, the amount of input information they demand exceeds the amount of predictive information they output. It was shown how to systematically construct quantum models that break this classical bound, and that the system of minimal entropy that simulates such processes must necessarily feature quantum dynamics. This result hints that if quantum effects are accounted for, many observed phenomena could be significantly simpler than classically possible. Other implications of this results are also discussed.

Tools of mathematical, computational and statistical sciences are also important for the development and support of experimental techniques and experimental nanoscience, including mathematics of quantum measurements and control of quantum systems. Nanophotonic approaches and dynamic measurements allow nowadays the visualization of dynamic processes on cell membranes with optical spatial resolution down to 30 nm and sub-millisecond time resolution [18]. These experimental techniques have led to new discoveries in cell biology, where one of the challenging problems is to understand the specific nanometer-scale organization. Among others, the authors of [18] mention the discovery of functional protein nanocomplexes that form under mechanical stress to activate cell signaling and cell adhesion. Mathematical models and new methodologies for analyzing adhesive and mechanical properties of complex nanosystems, in relation to function, have recently been discussed in [19].

1.6. Nanosystems in energy, environmental and other applications

Nanosystems play a key role in the development of alternative/renewable energy resources, including energy conversion, storage and harvesting. Some of the areas of interest at the nanoscale include solar cells, photovoltaics, and nanogenerators.

Nanoscale materials, nanoparticles, and nanocomposites are used in the design of devices and systems (e.g., nanosensors) for monitoring environmental conditions of ecological systems, soil, water, and air contamination. On the other hand, the dynamics of airborn nanoparticles and nanomaterials is often itself is a subject of environmental concerns. The development of mathematical models in these areas leads to challenging problems that are at the forefront of applied mathematics and numerical analysis.

As examples of emerging areas of nanoscience and nanotechnology, where mathematical models are at the beginning of their development, we mention nanoneuroscience, regenerative medicine and their applications and, at a large extent, food, agricultural and nutrition sciences, among others [20]. For example, interesting new directions include the problems of modeling properties of new food products after introducing nanoparticles for increasing bioavailability of food components.

2. Overview of the Inaugural Volume and Forthcoming Articles

Nanoscale Systems MMTA had a successful year. The inaugural volume of the journal contains 10 articles from some of the leading researchers in their respective fields. The volume is opened by the article from the group of Prof. C. Fong of the University of California, Davis. The authors review one of the important directions in spintronics. They discuss the development of new semiconductor-based magnetic materials for device applications using spin, or spin and charge, focusing on making use of materials involving Si, or more specifically on Si-based half metallic spintronic materials [21]. They provide details of (a) relevant experimental growth techniques, (b) the non-spin-polarized and spin-polarized forms of density functional theory, along with mathematical models based on the Kohn-Sham equations. Computational techniques to handle the associated models are also discussed, based on two software packages. Theory, mathematical modeling and computational techniques for this important direction in spintronic applications are explained in the context of recent design of half metallic quantum structures.

A group of researchers from the Reykjavik University, University of Iceland, and Clemson University in the USA in their article [22] presented an innovative analysis of interacting electron systems confined inside semiconductor quantum wires with spin orbit interaction in the presence of an external magnetic field. Their focus has been on the charge and spin distributions induced in such interacting systems. The mathematical models used for their analysis are based on the Hartree-Fock approximation of the many-body Hamiltonian problem, where they also account for the spin-orbit

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

coupling. Three different materials have been analyzed with the developed computational technique: GaAs, InAs, and InSb. The authors demonstrated that the influence of the Coulomb interaction on the electronic states depends on the material parameters of the heterostructure where the quantum wire is grown [22]. The important practical consequence of their analysis for a range of different applications lies with the fact that this interaction may amplify or modify the spin current.

Another research paper of the volume aims at better understanding of the thermal-transport properties of nanodevices based on mathematical models accounting for nonlocal effects via non-Fourier heat equations [23]. Particular attention has been given to the problem of heat removal and consequent cooling of nanosystems heated by some external sources (static or generated by fast laser pulses). Computational experiments have been carried out for hot nanosystems cooled through a graphene layer.

The next research article is devoted to the analysis of signals generated in memristive circuits consisting of nanostructured elements [24]. Such signals may have hysteretic distortion due to nonlinear and charge-dependent resistance (memristance). The author has demonstrated that such signals can be numerically represented in specially-designed nonorthogonal bases and this can be efficiently done with a numerical algorithm requiring only $O(NlogN)$ arithmetic operations. The author also elaborates on modeling hysteretic distortions of such signals with fast numerical transforms.

A review paper [25] provides a comprehensive discussion of mathematical models based on the nonparabolic effective-mass approximations and their applications to the study of semiconductor quantum dots. Both single electron models and many-electron models are discussed, as well as configuration interaction and current-spin density functional theory approaches. A major focus is given to the models resulting after discretization in nonlinear eigenvalue problems. A range of suitable methods for numerical treatments of such problems is discussed with numerical examples, emphasizing the issues related to accuracy of the models, physical novelty, and efficiency of nonlinear eigensolvers. These issues are discussed in the context of relevant experimental data.

In the research article [19] the authors deal with inverse problems in nanomechanics. In particular, they are interested in quantification of several important material parameters for application of theories of adhesive contact to nanomechanics, namely in the effective elastic modulus of contacting solids and the work of adhesion. Their developed methodology is based on a single test using a non-direct approach founded on an inverse analysis of a stable region of the force-displacements curve obtained from the depth-sensing indentation of a sphere into an elastic sample. Advantages of the proposed method are discussed and its robustness is demonstrated by its application to soft polymer (polyvinylsiloxane) samples. Other aspects related to the solution of associated inverse problems for adhesive contacts and experimental evaluations of material properties for nanomechanics applications are also discussed.

It is well known that the control of quantum systems represents one of the most challenging problems of modern science. It is a central problem in applications of quantum mechanics. In the article [26], the author focuses on this problem from a mathematical perspective, motivated by the fact that it appears in a variety of present and perspective applications ranging from quantum optics and quantum chemistry to semiconductor nanostructures, including the emerging fields of quantum computation and quantum communication. The major focus of his article lies with adjoint methods and their numerical implementation in the context of optimal control of quantum systems. Both finite and infinite dimensional quantum systems are discussed and an outlook to future developments is given.

Along with traditional microscopic approaches based on the Boltzmann equation, new applications in micro and nanoelectronics have led also to an increasing interest in macro and mesoscopic approaches and in associated mathematical models based on generalized transport equations that include memory and nonlocal effects. In the article [27], the authors review some of the most important phenomena due to the phonon-wall collisions in nonlocal heat transport in nanosystems, and show how they may be described through certain slip boundary conditions in phonon hydrodynamics. The treatment of these phenomena is demonstrated with the developed mathematical models on a number of examples quantifying heat conduction in nanowires of different cross sections and in thin layers. Among other effects important at the nanoscale, the authors consider thermoelectric effects.

The development of nanosystems for medical applications represent an important avenue of research in nanoscience and nanotechnology. Mathematical modeling techniques substantially contribute to this development. In the article [28], the authors presented a comprehensive review of ion channel based biosensors with their major focus on the mathematical modeling of the state-of-the-art ion channel switch (ICS) biosensor and the novel cation specific (CS) sensor. Biosensors, discussed in this article, have applications in the fields of medicine, engineering, and biology. Furthermore, due to their high sensitivity and rapid detection rates, they are becoming an attractive option for biomimetically engineered nanomachine devices capable of measuring femto-molar concentrations of chemical species and the detection

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

of channelopathies (ion channel disorders). Based on ordinary and partial differential equations, the authors of [28] demonstrate how to determine a range of important characteristics of such biosensors, including the characteristics of the analyte present in the electrolyte, the ionic transport of chemical species, and the bioelectronic interface present in the ICS biosensor and CS sensor. The methodologies presented are important for modeling similar bioelectronic devices. In addition to the continuum mathematical models for the ICS and CS sensors, the authors also presented methods by which first-principle approaches can be used to obtain macro-level parameters such as conductance and chemical reaction rates. Particular attention was given to the methods based on a combination of molecular dynamics techniques with stochastic methodologies.

Statistical modeling, which includes Monte Carlo, Markov Chain and Bayesian techniques, is an important tool in nanoscience research. The article [29] discusses the application of this tool to study nanomaterials. Due to their unique properties, nanomaterials have a great potential in applications ranging from electronics, sensors and solar cells to super-strong materials and coatings, from drug delivery and nanomedicine to their applications in improving the the environment by detecting, preventing and removing pollutants. They also bring new challenges and the authors of [29] focus on one of such challenges connected with the precise control of the morphology of nanomaterials, which is critical to the development of advanced nanodevices with various functionalities. This task is exemplified in the paper by the analysis of one-dimensional CdSe nanostructures focusing on the synthesis of such nanostructures whose morphologies are represented by nanowires, nanobelts, and nanosaws. The authors apply existing Bayesian methodologies to describe the growths of these nanostructures in terms of process variables and to predict the probability of transition from one nanostructure to another when changes are made to one or more process variables. They propose a Bayesian algorithm to identify the optimal process conditions that maximize the predicted probability of each type of nanostructure.

A number of exciting articles are forthcoming shortly in 2013. Among them we will mention articles [30] and [6]. In [30], by using atomistic calculations, the authors determine the eigenmodes and the vibrational properties of the ground state configuration of graphene clusters. Based on their developed technique with the modified Brenner potential, they have also described the carbon-carbon interaction and carbon-hydrogen interaction in the case of H-passivated edges and calculated the specific heat of the clusters within the harmonic approximation. In the article [6], the authors provide a review of graph theoretical approaches to modeling nanoscale systems, focusing on the analysis of the structure and dynamics of complex systems at nanoscale. Many interesting examples have been provided to illustrate these approaches, including examples of bionanosystems, as well as examples of nanoparticle networks modelling complex nanomaterials.

3. NanoMMTA Readership and Invitation to Contribute

The NanoMMTA journal offers a stimulating exchange of ideas for members of different scientific, engineering, and mathematical communities, who are involved in studies, developing, manufacturing and applications of nanoscale systems, to foster extensive interdisciplinary collaboration in this multidisciplinary field. The readership of the journal ranges from scientists and engineers, who develop new nanoscale-based technologies, to biomedical and life science professionals, and to physicians, who are interested in the application of such technologies.

This international peer-reviewed journal aims to connect and consolidate research activities in all aspects of nanoscale systems where the application of mathematical, computational and statistical tools is becoming increasingly important. Publishing full research papers, state-of-the-art reviews and short communications which are encompassing both the fundamental and applied research, the NanoMMTA journal covers a broad range of topics that are of interest not only to specialists in their respective research areas from academia, industries and government laboratories, but in a number of cases also to policy makers who are interested in the most recent developments in nanoscale systems. Enabling and promoting interactions between its diverse readership community, the NanoMMTA journal will strive to be a prime forum for communicating innovative research results in nanoscale systems at theoretical, computational and experimental levels, developing new opportunities via multidisciplinary collaboration, and opening up new ways for significant advances in this rapidly evolving field.

The NanoMMTA may occasionally publish topical/special issues. Perspective guest editors, that may include organizers of relevant conferences, are welcome to contact us to discuss such projects. Please note, however, that we do not publish conference proceedings per se. Papers must be prepared in one of the article categories published by regular issues of the NanoMMTA journal. There are no limits in manuscript volume for survey/review and research articles in such topical/special issues. Short communications can also be part of such issues, provided they satisfy the requirements for Rapid Communications (NanoMMTA Letters) of the journal (http://www.degruyter.com/view/j/nsmmt). All papers submitted to such issues will go through the NanoMMTA high standard and comprehensive peer-review

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

procedure. The primary criteria for judging the acceptability of manuscripts in topical/special issues remains their originality, scientific importance and interest to a general audience working in diverse areas of nanoscale systems and their applications.

Our regular submissions include all three categories mentioned above, Full Research Papers, Survey Articles, and NanoMMTA Letters. We would hereby like to invite you to contribute to the NanoMMTA journal and we look forward to receiving high quality manuscripts from you in any area covered by this journal.

References

[1] A. V. Antoniouk and R.V.N. Melnik. Scientific frontiers at the interface of mathematics and life sciences. *Mathematics and Life Sciences*, De Gruyter, Berlin, New York, pp.1–16 (2012).

[2] R.V.N. Melnik and I. S. Kotsireas, Interconnected challenges and new perspectives in applied mathematical and computational sciences. *Advances in Applied Mathematics, Modeling, and Computational Science, Fields Institute Communications* **66**, Springer, New York, pp. 1–10 (2013).

[3] K. Tai, M. Dao, S. Suresh, A. Palazoglu, and C. Ortiz. Nanoscale Heterogeneity Promotes Energy Dissipation in Bone. *Nature Materials*, **6**, 454–462, (2007).

[4] L. Adler-Abramovich, D. Aronov, P. Beker, M. Yevnin, S. Stempler, L. Buzhansky, et al. Self-assembled arrays of peptide nanotubes by vapour deposition. *Nature Nanotechnology*, **4 (12)**, 849–854 (2009).

[5] H. Q. Shi, A.S. Barnard, and I.K. Snook. Quantum mechanical properties of graphene nano-flakes and quantum dots. *Nanoscale*, **4 (21)**, 6761–6767 (2012), DOI: 10.1039/c2nr31354e.

[6] J. Zivkovic and B. Tadic. Nanonetworks: The Graph Theory Framework for Modeling Nanoscale Systems. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **2**, 30 (2013), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2013-0003.

[7] N. O. Weiss, H.L. Zhou, L. Liao, Y. Liu, S. Jiang, Y. Huang, et al. Graphene: An Emerging Electronic Material. *Advanced Materials*, **24 (43)**, 5782–5825 (2012), DOI: 10.1002/adma.201201482.

[8] L. Cademartiri, K. J. M. Bishop, P.W. Snyder, and G.A. Ozin. Using shape for self-assembly. *Philosophical Transactions of the Royal Society A - Mathematical Physical and Engineering Sciences*, **370 (1969)**, Special Issue: SI, 2824–2847 (2012), DOI: 10.1098/rsta.2011.0254.

[9] R.V.N. Melnik and A. Povitsky, editors. Modelling coupled and transport phenomena in nanotechnology. *Journal of Computational and Theoretical Nanoscience*, **3 (4)** (2006).

[10] S. Prabhakar, R. V. N. Melnik, P. Neittaanmaki, and T. Tiihonen, Coupled electromechanical effects in wurtzite quantum dots with wetting layers in gate controlled electric fields: The multiband case. *Physica E: Low-dimensional Systems and Nanostructures* **46**, 97–104 (2012).

[11] S. Prabhakar, R.V.N. Melnik, P. Neittaanmaki, and T. Tiihonen, Coupled magneto-thermo-electromechanical effects and electronic properties of quantum dots. *Journal of Computational and Theoretical Nanoscience* **10**, 550–563 (2013).

[12] P. Tiwary and A. van de Walle. Hybrid deterministic and stochastic approach for efficient atomistic simulations at long time scales. *Physical Review B*, **84 (10)**, 100301 (2011) DOI: 10.1103/PhysRevB.84.100301.

[13] M. Paliy, R. Melnik, and B. A. Shapiro. Coarse-graining RNA nanostructures for molecular dynamics simulations. *Physical Biology*, **7 (3)**, 036001 (2010).

[14] A. Cambi and D.S. Lidke. Nanoscale Membrane Organization: Where Biochemistry Meets Advanced Microscopy. *ACS Chemical Biology*, **7 (1)**, 139–149 (2012), DOI: 10.1021/cb200326g.

[15] D. R. Han, S. Pal, Y. Liu, H. Yan. Folding and cutting DNA into reconfigurable topological nanostructures. *Nature Nanotechnology*, **5 (10)**, 712–717 (2010), DOI: 10.1038/nnano.2010.193.

[16] D.N. Kim, F. Kilchherr, H. Dietz, and M. Bathe. Quantitative prediction of 3D solution shape and flexibility of nucleic acid nanostructures. *Nucleic Acids Research*, **40 (7)**, 2862–2868 (2012), DOI: 10.1093/nar/gkr1173.

[17] M. Gu, K. Wiesner, E. Rieper, and V. Vedral. Quantum mechanics can reduce the complexity of classical models. *Nature Communications*, **3**, 762 (2012), DOI: 10.1038/ncomms1761.

[18] Y. F. Dufrene and M.F. Garcia-Parajo. Recent progress in cell surface nanoscopy: Light and force in the near-field. *Nano Today*, **7 (5)**, 390–403 (2012), DOI: 10.1016/j.nantod.2012.08.002.

[19] F.M. Borodich, B.A. Galanov, S.N. Gorb, M.Y. Prostov, Y.I. Prostov, and Suarez-Alvarez, M.M. An inverse problem for adhesive contact and non-direct evaluation of material properties for nanomechanics applications. *Nanoscale*

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM

Systems: Mathematical Modeling, Theory and Applications, **1**, 80–92 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0006.

[20] P. R. Srinivas, M. Philbert, T.Q. Vu, Q. R. Huang, J.L. Kokini, E. Saos, et al. Nanotechnology Research: Applications in Nutritional Sciences. *Journal of Nutrition*, **140 (1)**, 119-124 (2010), DOI: 10.3945/jn.109.115048.

[21] C. Y. Fong, M. Shaughnessy, L. Damewood, and L. H. Yang. Theory, Experiment and Computation of Half Metals for Spintronics: Recent Progress in Si-based Materials. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 1–22 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0001.

[22] H.A. Thorolfsson, A. Manolescu, D.C. Marinescu, and V. Gudmundsson. Coulomb interaction effects on the spin polarization and currents in quantum wires with spin orbit interaction. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 23–37 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0002.

[23] A. Sellitto and F.X. Alvarez. Non-Fourier heat removal from hot nanosystems through graphene layer. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 38–47 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0003.

[24] A. Sowa. Signals generated in memristive circuits. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 48–57 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0004.

[25] J.-L. Liu. Mathematical modeling of semiconductor quantum dots based on the nonparabolic effective-mass approximation. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 58–79 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0005.

[26] A. Borzi. Quantum optimal control using the adjoint method. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 93–111 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0007.

[27] F.X. Alvarez, V.A. Cimmelli, D. Jou, A. Sellitto. Mesoscopic description of boundary effects in nanoscale heat transport. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 112–142 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0008.

[28] W. Hoiles, V. Krishnamurthy, B. Cornell. Mathematical Models for Sensing Devices Constructed out of Artificial Cell Membranes. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 143–171 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0009.

[29] N. Ebrahimi, M. Shehadeh, K. McCullough. Bayesian Analysis for Robust Synthesis of Nanostructures. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **1**, 172–186 (2012), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2012-0010.

[30] S. K. Singh and F. M. Peeters. Vibrational Properties of Nanographene *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, **2**, 10–29 (2013), ISSN (Online) 2299-3290, DOI: 10.2478/nsmmt-2013-0002.

Unauthenticated | 99.229.2.100
Download Date | 9/16/13 2:14 AM