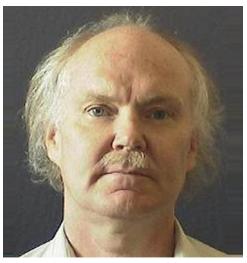
# Preface

# (A Historical Prespective) to CPC's 6th Year, 2016 (A New Beginning)



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The 2016 marks the sixth year of *Current Physical Chemistry* (CPC) with volume 6, issue 1. In the past five years, CPC has continued to grow, mature, and expand as a high quality physical chemistry journal and has established itself as a truly diverse and unique publication among the many peer reviewed physical chemistry journals. In 2016 and in the foreseeable future, it will maintain this uniqueness and continue to publish high quality reviews and research articles in the diverse areas of physical chemistry, biophysical chemistry, chemical physics, biotechnology, and quantum nanobiology.

In 2013 CPC published several Special Issues, including two on Quantum Nanobiology and Biophysical Chemistry, one on the Synthesis and Application of Graphene Based Nanomaterials, and finally Part I of the Structure-Property Relationships of Ceramics, Nanotubes, and other Advanced Materials. In addition, the journal also published a number of separate research, review, and feature articles within these four special issues. These publications covered many interesting topics in physical chemistry, in particular, the physics and chemistry of nanomaterials, which are of increasing importance in nanoscience and nanotechnology, all of which are based on a thorough understanding of physical chemistry, biophysical chemistry, and chemical physics.

Over the past few years, the boundaries of Science, including Physical Chemistry, have expanded beyond one's wildest imaginations (at least most people's imaginations).

In the first issue of 2014, Part II of the special topic of Structure-Property Relationships of Ceramics, Nanotubes, and other Advanced Materials, edited by Carlton Taft, was published which documented a good example, covering topics ranging from photoluminescence in $PbMoO_4$ and $SrSnO_3$, pharmacophore-based drug design for Alzheimer's disease, to doped solid oxides for fuel cells, and electronic structures of dioxoosmium complex ions. It also covers general articles on protein aggregation by Saha and Deep, and molecular packing of conjugated compounds of carbazole acrylonitrile derivatives by Percino *et al*. just to name a few.

In the second issue of 2014, the diversity of research being done by physical chemists was shown by the works of Batista/Coutinho/Gomes, Pandey/Rai, Rahim/Jalkanen, and Li/Guan/Yang on i) Prediction of Ionic Liquid Properties though Molecular Dynamics Simulations, ii) Theoretical Prediction of Thermal Pressure for Geophysical Minerals, iii) Protein Interactions, Hydration, and Solvation Structure of Osmolyte Solutions: Lysozyme in Free Amino Acid Soutions, and iv) a Computational Revew of Olefin Metathesis over Mo-exchanged Zeolites. In addition, a review of recent patents and highlights of functionally engineered nanoparticles for applications in biology, medicine and nanomedicine was published. Here the next phase of the scientific endeavor is being advocated and published, that is, Translational Research, that is applying fundamental biophysical, chemical and physical chemistry to solve problems in society, and this includes patenting one's work when there are socioeconomic consequences/applications of one's discoveries, research and technologies.

In the third issue of 2014 (issue 3, volume 4) I was introduced as the new Editor in Chief of CPC taking over from Professor Ruhong Zhou at Columbia University (Department of Chemistry) and IBM Thomas J. Watson Research Center (Computational Biology Center). In this issue Editorial Board member Professor Ricardo Tucceri contributed an impedance study on the effects of pH on electron transport rates at poly(o-aminophenol) film electrodes, a work in nanosensor/nanotechnology development. Other contributions in this issue included the work of Inamoto/Kurihara/Yajima on electrode performance of sulfur-doped vanadium pentoxide gel prepared by microwave irradiation for rechargeable magnesium batteries, and others works on the hysteresis of mixed monolayers, a review on recent progress in perovkite oxide based thermoelectric materials, a study on length-dependent magnetoresistence in aromatics matereitals, a studies on the kinetics and mechanism of i) electron transfer reactions and ii) oxidation of paracetamol.

In the fourth and final issue in 2014 Professor Mehmet D. Turan guest edited a thematic issue titled: Alternative Metal Production Methods, Modeling, and New Reaction Suggestions. In this special issue Turan/Kalender published an alternative approach for metal production from copper slag and Karip/Muratoglu/Aydin published a method to produce new metal coupled with Al alloys $Ni_3Al$ composites using diffusion welding, a work which combines the fields of physical chemistry, chemical engineering and physical metallurgy. Lupi/Dell'Era/Pasquali published a nice work on recycling and the production of Ni-Co alloys from secondary spent batteries by electrotwinning. Finally, Professor Peter I. Nagy published a comprehensive review article on structure simulations of small organic molecules in solution at ambient temperatures and neutral pH.

2015 marked the 5$^{th}$ year of CPC with another thematic issue titled: Self-Organizatoin in Active Soft Matter edited by Professor Takahiko Ban. This issue included works on the Liesegang phenomena by Nabika, self-propelled objects in response to their environment by Suematsu/Nakata, the design of reactive surfaces by Banno/Toyota, the viscous fingering phenomena by Nagatsu, fluctuations and responses in stochastic motions in Volvox colonies by Ozaki/Murayama, self-propelled particles with rotational asymmetric shapes by Nagai/Hayakawa/Takinoue, coupling between a chemical wave and motion by Miyazaki/Sakurai/Kitahata, and finally directed propulsion, chemotaxis and clustering in propelled microparticles by Duderdale/Ebbens. In this special issue, the effects of both the chemical environment, shapes of molecules and the velocities/momenta were all considered, the field of reactive chemical fluid dynamics. In many cases, the momenta/shapes/motions have not been considered in chemical reactions, but with the Nobel Prize by Zuwail on reactive scattering, the need to address these issues have now become topics of fundamental research by top groups in Japan and in many other countries. The merger of chemical engineering, computational fluid dynamics and physical chemistry has never been larger. The late Professor Arthur Adamson, the author of the classical Physical Chemistry text used at many technical universities, initiated a journal especially for surface science in chemistry. CPC welcomes submissions in multidisciplinary areas of science and technology which do not yet have specialty journals, the theme of Professor Ban's special issue being just one example.

In the second issue of 2015, Senda and colleagues published a theoretical investigation of field emission of aligned carbon nanotubes, Kolel-Ventil *et al.* published a work investigation on how to stabilize metastable W2C nanoparticles, Gun'ko published a work on the effects of confined space (capillary and tubular confinement and flow) and the structure of adsorbents on the behavior of polar and non-polar absorbates at low temperature, and finally Posati *et al.* published an overview article on different approaches to obtain luminescent hydrotalcite nanoparticle and films. Again set of multidisciplinary contributions by researchers thinking and workout side of the standard box/paradigm of physical chemistry.

In the third issue in 2015, Carlton Taft edited Part III of his thematic set of issues on Ceramics, Nanotubes and Materials. Qui/Bi/Liu published a work on the fabrication and characterization of solid oxide fuel cells, Topaz *et al.* published a review article on identifying lead compounds with increased specificity and potency in the field of drug design, Silva *et al.* published a comparison of experimental and theoretical structural and electronic data used to characterize chitin and chitosan, Lucena *et al.* published a facile synthesis method to obtain $SrSnO_3@AK_2$ (A=Ti or Zr) core shell systems, Canchaya/Furtado/Taft published an overview of fuel cells and simulation models, Federico *et al.* published a ligand structure based drug design strategies for screeing BACE1 inhibitors, and finally Lacerda *et al.* published a KS-DFT investigation of sulfur doping on ZnO materials.

In the last issue of 2015, Mammino contributed a KS-DFT investigation of chinesin I and II, Figueredo *et al.* contributed an investigation of acetylcholinerase inhibitors based on piperine and its acid and ester derivatives, Andrade *et al.* contributed an investigation on the PEDOT polymeric chains, Tesfay *et al.* contributed an investigation of the effects of heptamethine iodine and heptamethine $PF_6$ solutions on the measurements of low dose X-ray and gamma radiation, Silva *et al.* contributed a comparative study of the effects of Nd doping on SrTiO3 films, Marana *et al.* contributed a theoretical investigation on the band alignment mechanism for the ZnO@ZnS interface of core-shell structures, and finally Oliveira /Martins contributed a theoretical study on focal adhesion kinase inhibitors.

Finally to the first two issues of 2016, the 6th year of CPC. In the January and April 2016 issues of CPC, Carlton Taft has co-edited Parts V and VI of his continuing thematic set titled: Ceramics, Nanotubes and Materials. In part IV, Silva *et al.* have contributed simulation study on the analysis of titanium oxide nantubes with the rutile and anatase structures, Ribeiro *et al.* have contributed a study of band gap engineering based on anionic and cationic doping of $TiO_2$ anatase, Santos *et al.* have contributed a modeling study NS3 protease inhibitors of the type 2 Dengue virus, Ribeiroa/Lazaro have contributed an ab initio study of the structural and electronic properties of ilmenite-type $FeGeO_3$, Silva *et al.* have contributed a theoretical study of gallium arsenide nanotubes, Souza el al. have contributed a work on the development of monoamine oxidase B inhibitors for the treatment of Parkinson's disease, and finally Lacerda *et al.* have contributed a KS-DFT theoretical study on the influences of Ba-doping on the ferroelectric, optical and electronic properties of wurtzite ZnO.

We envision more such high-quality publications with broad interests in the forthcoming issues. Bentham Science and I also hope that authors will find CPC a suitable platform to publish their great findings for the benefit of the entire scientific community, especially multidisciplinary areas where physical chemists have worked outside of the box, the conventional paradigms and worked in areas of applied, application, and translational research which involves extending and applying fundamental physical chemistry concepts, theories and methodologies in areas and space where no physical chemists have gone before, or at least very few.

Finally, I would like to take this opportunity to thank Bentham Science for appointing me as Editor-in-Chief (EiC) of the journal, and Ms. Raheela Anjum, Ms. Noureen Azhar, Ms. Iqra Nasim, Mr. Muhammad Jawad Iqbal and Ms. Narmeen Khurram for their enthusiasm, dedication and support. I would also like to thank all our referees for their precious time and expertise and the number of Guest Editors of special issues of CPC, especially Dr. Carlton Taft in Brazil for his 6 part thematic issue set. Along with recently hosting the World Cup in soccer where Brazil reached the semifinals, Brazil this summer is hosting the Olympics. In addition to funding both soccer and many Olympic sports to the highest level, Brazil and its States are also funding fundamental and applied research via CAPES (Federal Government) and FAPESP (State of Saõ Paulo). We encourage other South American and African countries' physical chemistry researchers to use Current Physical Chemistry as their main journal for publication of their unique and diverse chemical, petroleum, pharmaceutical and medical chemistry research based on high level physical chemistry, mathematics, statistics, molecular biology, quantum nanobiology, biophysical chemistry, and chemical physics. These countries have relatively young (in-age) populations with many young scientists who need nurturing and maturing, just like a relatively young journal like CPC. Our goal at CPC is to not only publish high quality reviews and research articles, but to be a medium where young researchers, MSc, MBt, PhD and postdoctoral students can submit their work for peer review, get positive, rigorous and tough peer reviews which will allow them to improve upon their work, and after appropriate (major) revision, publish their work. Hence we are most grateful to the large number of very conscientious tough referees who have not only been willing to review their colleagues' work, but also many of whom also have been willing to "mentor" their colleagues through the peer review process, and not only the young researchers and scientists, but in some cases even their young research advisors who themselves are in the early stages of their research and/or academic careers. But this is not to say a scientific work should be submitted for publication to CPC in too rough a state, before it is scientifically mature and ready, just that CPC is much more likely to ask for major revision and allow a considerable amount of time for the authors to undertake at the revision stage, than most journals (which have high rejection rates and in many cases are not even willing to send out works for peer review). Coming from an applied mathematics and chemical physics background, one realizes that to do fundamental work and review fundamental works of others in a rigorous review, takes not only time, but in many cases very rigorous and critical comments and queries from one's scientific colleagues (and peers), who are also interested in raising the bar and quality of the scientific endeavors not only theirs, their groups, at their host institutes, countries and regions, but throughout the globe. By helping others, we ultimately help ourselves. We pride ourselves in publishing works from all continents and countries, focusing on the young and growing South American, African, Asian, Middle Eastern, and Euroasian countries, many of which have recently changed over from

one type of socioeconomic model to another, which itself has resulted in very large number of growing pains in not only the economics of these countries and regions, but also in the scientific endeavor, the Balkans, Afghanistan, Libya, Syria, Iraq, Serbia, Kosovo, Ukraine and Crimea to name a few, Kosovo and Crimea being the latest two countries to be welcomed to the countries, the researchers of which are encouraged to publish their fine works in CPC.

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