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CONDENSED MATTER PHYSICS

Foreword

Computer simulations of soft matter. On 60-th anniversary of Jaroslav Ilnytskyi

This special issue Condensed Matter Physics, entitled "Computer Simulations of Soft Matter" is dedicated to Jaroslav Ilnytskyi on the occasion of his 60-th birthday. Prof. J. Ilnytskyi is one of scientific leaders of the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine (NASU), who is well known for his contributions to the theory and computer simulation studies of polymer fluids, liquid crystals, macromolecular and colloid solutions. Versatility of Jaroslav works is due to his excellent background commonly resulting in original ideas, his feeling and ability to choose and apply appropriate methods for the solution of various problems. Finally, Jaroslav works are distinguished by the profound analyses of either theoretical or simulation results with respect to experimental observations frequently complemented by the discussion of possible applications. It seems that the contributions by J. Ilnytskyi have a certain artistic touch, since he was lucky to be trained at the school age as a violin player, next he mastered several other musical instruments and shares this activity with science permanently. J. Ilnytskyi published over 130 papers in highly prestigious journals, several review articles and book chapters.

Jaroslav Ilnytskyi was born on October 7, 1963, in Lviv. In 1980 he entered the Physics Department of the Ivan Franko National University of Lviv. Jaroslav graduated from the University and obtained a master degree with honors in 1985. In the same year, he entered the postgraduate studies at the Lviv Division of Statistical Physics of the Institute for Theoretical Physics in Kyiv. In 1990 this Division was transformed into the Institute for Condensed Matter Physics (ICMP). J. Ilnytskyi received the PhD degree in physical and mathematical sciences having defended the dissertation "The Method of Collective Variables and ε-expansion" at the Ivan Franko National University of Lviv (1994). His scientific mentor was Prof. I. Yukhnovskyi, the founder of the Lviv school of statistical physics. Principal issues of the research within this area have been discussed in [1, 2]. In essence, the main goal of these studies was in the construction of effective combination of the collective variables method by I. Yukhnovkyi and

K. Wilson's renormalization group approach. Along this strategy, the authors intended to describe the second-order phase transition with universal characteristics like critical indices, together with explicit results for thermodynamic and structural properties near the phase transition point. Jaroslav Ilnytskyi preserved admiration by the phase transition problem throughout his subsequent carreer.

After the PhD degree, J. Ilnytskyi was looking for extensions of his knowledge to new research areas and to explore novel methodological tools. Specifically, physics of liquid crystals and computer simulations methods has attracted his attention. Perfect illustration of a successful start of his activities is given in [3], that describes Monte Carlo simulation study of nematic-isotropic phase transition within Lebwohl-Lascher model. At that time, one of us (O.P.) advised Jaroslav to visit the laboratory of Prof. Stefan Sokołowski at Maria Curie-Sklodowska University at Lublin in Poland. Lublin and Lviv are geographically quite close to each other. On the other hand, Ukraine had just started to find place within the existing European scientific structure in this decade. The visit of Jaroslav to Lublin in 1998 resulted in fruitful scientific colaboration during the following decades. At the very beginning, certain aspects of the problem of description of partly-quenched fluids were considered with success [4, 5]. In particular, changes of the nematic-isotropic transition in a lattice Berne-Pechukas type model were captured using Monte Carlo simulations complemented by histogram reweighting technique and finite size scaling analysis [5].

In 1998, J. Ilnytskyi participated in the first Erice school of Liquid Crystal Modelling, organized by C. Zannoni and P. Pasini (University of Florence, Italy) in Erice (Sicily). Very soon after this event Jaroslav was invited to take a postdoctoral position at the Chemistry Department of Durham University (Great Britain) in the laboratory of Prof. Mark Wilson. Jaroslav Ilnytskyi held this position from 1999 till 2003, dedicating to the studies of model liquid crystalline polymer systems using molecular dynamics and Monte Carlo computer simulations. Moreover, he contributed to the development of the novel parallel molecular dynamics code, known as GBMOLDD [6, 7]. Several important results within liquid crystals project were obtained in this period of time [8–11]. This set of valuable works provide a rather comprehensive description of the original computer simulation instruments designated specifically for liquid crystalline soft matter starting from simple models, e.g., a model liquid crystal dimer composed of two mesogenic units linked via a flexible alkyl chain [6] or nematic liquid crystal phase of one-site Gay-Berne molecules [7], to much more sophisticated systems, such as model dendrimer immersed in a mesogenic solvent of Gay-Berne particles, which can form nematic and smectic — a phases in addition to the isotropic liquid [10]. Moreover, in spite of the importance of technical tools, the principal focus is on physics and properties of the systems under study. Hence, the reader see a well established balance between tools and results of theoretical and practical importance. Apparently, the project resulted in several additional findings, see [12–15], besides the planned original purposes.

In 2004 J. Ilnytskyi returned to ICMP for a while. He was actively involved in the study of the critical behavior of the diluted lattice model of an N-component magnet using the cluster methods [16–18]. Undoubtfully, Jaroslav's experience in the application of Monte Carlo simulation techniques was crucial in analysis of the critical behaviour of the 3D quenched diluted Ising model considered in these publications.

Jaroslav belongs to theorists who fully appreciate the experimental knowledge of the systems they study. Therefore, he was looking for a place where frontier experimental research in liquid crystals and related polymer materials was developing. During 2005–2006 and in 2008, J. Ilnytskyi took a postdoctoctoral fellowship at Physics and Astronomy Department of the University of Potsdam (Germany) in the experimental laboratory of Prof. Dieter Neher. Ilnytskyi was assigned to work on the project on photo-induced deformations in azobenzene-containing polymers using molecular dynamics computer simulations. The starting point of this research, with D. Neher and M. Saphiannikova, was in elucidating the morphology, dynamics, and self-organization in side chain liquid crystalline polymers [19, 20]. In addition, J. Ilnytskyi in colaboration with Michael Allen [21] from the University of Bristol investigated the properties of liquid crystalline elastomers.

The azobenzene project has been developing quite fast, [22–27]. Originally it was thought as computer simulation investigation only. However, J. Ilnytskyi with his collegues, modified the initial aims and supplemented experimental outputs and simulation data by a solid theoretical background. Using fundamental kinetic equations for photoisomerization, it was shown that illumination by light can be reformulated as the action of an effective potential that determines orientation of the azobenzene chro-

mophores with respect to polarization direction. The strength of the effect principally depends on the refractive index and viscosity of the azobenzene containing materials [25].

In the meantime, in 2010, Jaroslav defended his second dissertation "Phase transitions in polymers and liquid crystals: computer simulations on different spatial and temporal scales" to obtain the habilitaion degree of Doctor of Physical and Mathematical Sciences. Patience, creativity, discipline and everyday hard work, besides talent, distinguish Jaroslav and lead him to success. In the following years, J. Ilnytskyi smoothly extended his research areas to inhomogeneous fluids, better say to inhomogeneous counterparts of many systems previously studied in the bulk. On the other hand, he learned and developed the programming tools to apply a dissipative particle dynamics (DPD) methodology, [28–30], appropriate to investigate off-lattice polymer models in a coarse-grained representation. As a result, new options to capture properties and phase behavior of several interesting systems appeared. The DPD method was implemented in Ilnytskyi's laboratory for different purposes. Initially, a microphase separation in melts of macromolecular amphiphilic molecules was investigated [31]. Next, a version of this kind of technique, in the form of mesoscopic and coarse-grained molecular dynamics, was applied to polymer and liquid crystalline brushes [32–37]. In addition, several methodological problems of coarse-grained type simulations for specific purposes were considered in [38–41]. It is next to impossible here to even mention the whole set of findings and principal results obtained within this ample research. An interested reader can consult original publications using links in the reference list to this foreword. However, certain summarizing insights are given in the review articles by Jaroslav and his co-workers, [23, 42, 43].

Still, it is worth mentioning a few projects from Ilnytskyi's laboratory under development at present. One of the challenging investigations with a possible impact on the material design of molecular brushes and membranes combines experimental research, computer simulation and some theoretical issues, [44–46]. Finally, Jaroslav exhibits a strong desire to design and apply mathematical models to medicine, e.g., epidemiology [47–50], and shows interest in drug delivery problems [51, 52].

During 2010–2023, J. Ilnytskyi was a principal investigator of a number of projects within the international cooperation programs, where he represented a Ukrainian side. In particular, he led the projects "Statistical Thermodynamics and Computer Simulations of Complex Moleculae in Bulk and at Surfaces" (2010–2014) within the FP7 program and "Structure and Evolution of Complex Systems with Applications in Physics and Life Sciences" (2014–2017) within the FP7-PEOPLE program of EU. He was a principal investigator of the joint Ukrainian-American project "Efficient Multi-enzyme Complexes for Cellulose Hydrolysis in Biofuel Production: experiments, theory and computer simulations" supported both by the CRDF Global and the Ministry of Education and Science of Ukraine within the USA-Ukraine Alternative Energy Research Competition program in 2020-2021 and the project "Smart surfaces for microalgae-based biofuel production" within the same program in 2022 supported seperately by the CRDF Global. These two latter projects were performed in a collaboration with Sergiy Minko (University of Georgia, USA). Among the national research programs it is worth mentioning that Jaroslav led the project "Computer modelling and theoretical approaches to describe the spread of the infectious disease COVID-19: the role of spatial heterogeneity of the population, heterogeneity of the network of social contacts and social feedback". This project was supported by the National Research Foundation of Ukraine within the framework of the program "Science for Human and Society Security" (2020–2021).

J. Ilnytskyi actively participates in teaching undergraduate and graduate students, in particular at the Department of Applied Mathematics of the Lviv Polytechnic National University, at the faculty of Aplied Sciences of the Ukrainian Catolic University. Under his supervision, four PhD students successfully defended their theses: A. Slusarchuk (2021), O. Kalyuzhnyi (2021), H. Ilnytskyi (2021) and D. Yaremchuk (2023). Since 2021, J. Ilnytskyi is the Head of the Department for Computer Simulation of Many-body Systems at ICMP. In 2022 he was awarded the title of professor. He received the medal of the Ukrainian Physical Society (2018) for original scientific results obtained in the field of photo-isomerization and the temporal evolution of molecular arrangement in azobenzene-containing polymer materials.

A contribution of J. Ilnytskyi in the fields of his scientific interests is essential and covers a study of a wide range of phenomena of theoretical, chemical physics and soft matter, specifically addressing the behavior of magnetic systems, liquid crystals, polymers and polymer brushes, and decorated nanoparticles. Despite the fact that the results obtained by J. Ilnytskyi principally concern fundamental science, several of them may find applications and contribute to technological advances.

This Special issue of Condensed Matter Physics features contributions from collaborators and friends of J. Ilnytskyi, focusing on contemporary challenges in soft matter and computer simulations. The guest editors, the entire editorial board of Condensed Matter Physics, and numerous friends in Ukraine and abroad extend their heartfelt congratulations to Jaroslav on his birthday. They warmly wish him to stay in good shape, and continue his active scientific life for many years.

Orest Pizio (Instituto de Quimica de la UNAM, Mexico, Mexico),
Taras Patsahan (Institute for Condensed Matter Physics, Lviv, Ukraine),
Viktoria Blavatska (Institute for Condensed Matter Physics, Lviv, Ukraine).

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