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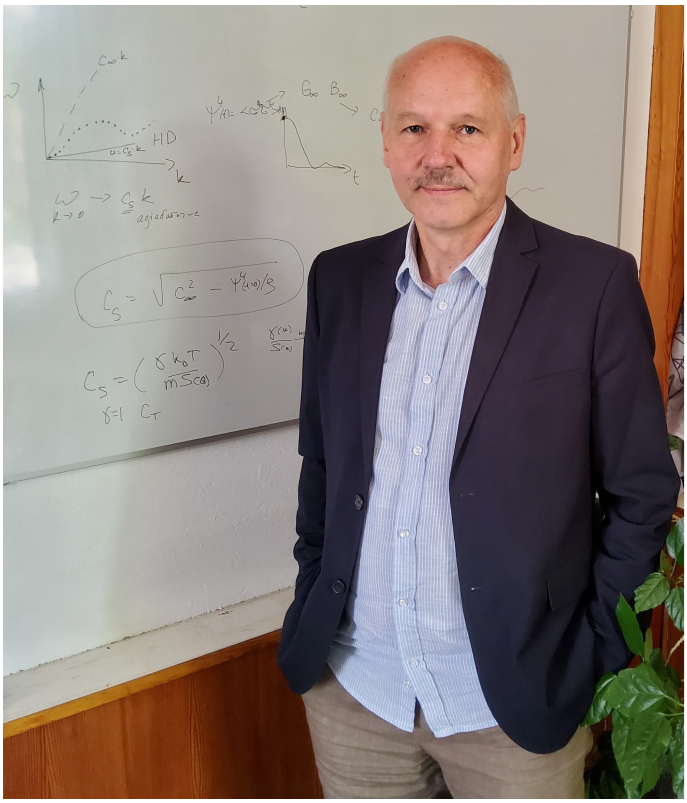
CONDENSED MATTER PHYSICS

Foreword

First-principles computer modeling and statistical theory in dynamics of liquids. On 60-th anniversary of Taras Bryk



In July 2023, our good friend and colleague Taras Bryk turns 60 years old. Today he is one of the leading experts in Ukraine and throughout the world in the field of first-principles and atomistic modeling of liquid metals and alloys, especially their dynamic properties and behavior under extreme conditions, and his scientific works are well cited and known among experts in the field. Since 2021, Taras Bryk is Director of the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine.

His first encounter with computing took place during his first year at the Faculty of Physics at Ivan Franko Lviv State University in the 1980s, during the so-called "stagnant times" in the USSR, when access to computing power was limited and the focus was mainly on military programs. Real writing and running computer programs started during the 1983 summer internship, when a group of students, including Taras Bryk, were given access to the computing facilities at the Institute of Physics in Kyiv for their practice in analyzing spectral data. In 1984–1985 Taras was working on his graduation thesis under the supervision of Yuri Myasoedov (now working at the Weizmann Institute in Israel), large share of which was based on computer calculations of surface electron states and capacity of the electrolyte-semiconductor interface. After graduation, he continued his research on the properties of semiconductors and metals at the University's Physics Department under the supervision of Marian Pashkovsky and

Ilya Talyansky (1985–1986). In February of 1987, he joined the Lviv Division of Statistical Physics (now the Institute for Condensed Matter Physics) of the Kyiv Institute for Theoretical Physics (now the Bogolyubov Institute for Theoretical Physics), founded and headed by Ihor Yukhnovskii at the time. Here he was actively involved [1] in the study of the electronic properties of metals in the group of Zinovij Gurskii, a well-known expert in the theory of pseudopotentials. A new and completely different experience became available to Taras thanks to the possibility of international internships. In 1993, he made his first research visit to the group of Karl Heinzinger (Max Planck Institute, Mainz, Germany), where he conducted computer calculations of the distribution functions for liquids and metallic ions in molecular liquids using molecular dynamics data. There he calculated structural factors and other properties of metal ions in ammonia.

In 1994, Taras Bryk defended his PhD thesis "A new method for studying the electronic structure of metals based on the formalism of fully orthogonalized plane waves" under the supervision of Z. Gurskii. After obtaining his PhD, Taras, seeking international scientific practice, went abroad to work in several fellowships and postdoctoral positions. The first fellowship from OeAD, the Austria's Agency for Education and Internationalisation, was at the Vienna Technical University (Austria) with Prof. Jürgen Hafner, one of the top experts in theory of metals and computer simulations. He encouraged Taras to use molecular dynamics simulations and focus on the complex dynamics of liquids and liquid metals [2], which determines a wide range of their physical properties. This area was also fruitfully developed [3–7] in Taras' active collaboration with Ihor Mryglod, which began in 1996 and continues till today, and was based on applications of the now well-known theory of generalized collective modes .

The first successes achieved in the field of computer simulations, allowed Taras Bryk to receive a two-year (1997–1999) postdoctoral fellowship in the group of Prof. Leonard Kleinman (Austin, Texas, USA), a true patriarch in the field of pseudopotential theory and *ab initio* modeling. The research topic concerned the magnetic properties of the surface of 4d-metals and required full parallelization of the *ab initio* code [8]. It was a great experience in writing parallel codes and running them on one of the most powerful supercomputers of the time, the Cray T3E. At the same time, Taras continued [9–11] to study the dynamic properties of liquid metals, combining the possibilities of computer simulations with a theory based on the formalism of generalized collective modes.

The next two years (2000–2002) Taras spent in Houston, in the same state, in the group of Prof. Anthony Haymet. Here, he focused [12–15] on simulations of the water-ice interface, ion hydration at the interface, and related research, which included complex water modeling, a problem that has fascinated researchers for decades and is still far from being finally solved. For this purpose, he used both classical and *ab initio* molecular dynamics simulations. Obviously, Taras saw in Anthony Haymet an example of both a prolific scientist and an effective manager, and perhaps at this stage he realized that both activities are in fact closely intertwined and can be combined with great success.

After returning to the Institute of Condensed Matter Physics in 2002, Taras continued his research in dynamics of liquids [16–23] (together with I. Mryglod). This resulted in a number of important publications and the defense of his dissertation thesis "Microscopic theory of kinetic collective excitations and their manifestations in the dynamics of simple and binary liquids" (for habilitation degree) in 2005. Taras' experience allowed him to work on other problems at the same time. Thus, in collaboration with the group of Prof. Myroslav Holovko, he studied the processes of hydrolysis and hydration in aqueous solutions of electrolytes [24–26]. Using molecular dynamics methods, this group studied the peculiarities of the structure of hydrated cations depending on their charge, which is important, in particular, for understanding the processes that occur when materials with radioactive elements come into contact with water.

Taking into account the relevance of the topic and the growing role of computer modeling methods in physical research, Taras Bryk was soon appointed Research Vice-Director of the Institute (2006) and Head of the newly created Department of Computer Simulations of Many-Particle Systems (2007).

Since then, the previous areas of his research, related, in particular, to the study of optical-type excitations in mixtures [27–33] and slow non-hydrodynamic processes [34–37], have been supplemented by the problems of the dynamic transition from gaseous to liquid-like behaviour in supercritical fluids [38–42], the influence of spatial constraints and type of interactions on the dynamics of fluids [43–47], the study of the properties of condensed systems under extreme conditions (high pressures and temperatures) [48–59] and applications of *ab initio* simulations to the description of very specific effects in condensed soft

matter [60–66]. The number of professional ties with the colleagues worldwide have also considerably increased. In particular, beside the authors of this foreword, Taras Bryk actively cooperates with Tullio Scopigno (Sapienza Universita di Roma), Jean-François Wax (Université de Lorraine, Metz, France), Anatoly Belonoshko (Royal Institute of Technology, Stockholm, Sweden), Noel Jakse (Université Grenoble Alpes, CNRS, Grenoble, France), Ari Paavo Seitsonen (Ecole Normale Supérieure de Paris, France), and others.

Taras is the author of more than 300 scientific works, some of them being listed at the end of this article. He takes an active part in a number of scientific organizations and structures both in Ukraine and abroad. In 2017–2020 he was a representative of Ukraine in the program committee for infrastructure projects of the European program Horizon-2020, a member of the expert council of the State Attestation Commission of Ministry of Education and Science of Ukraine for physical disciplines, the deputy editor-in-chief of the journal "Condensed Matter Physics", a member of the editorial board of the journals "Metallophysics and Advanced Technologies" and "Progress in Physics of Metals", a member of the international committee Liquid and Amorphous Metals (LAM). Considerable attention is paid to the work with students and young scientists. He is a professor of the chair of applied physics and nanomaterials of the Lviv Polytechnic National University; as an invited professor he worked at the University of Rome La Sapienza (2012, 2019) and University of Lorraine (2010, 2015). In the Institute for Condensed Matter Physics he is the chief of the scientific and educational doctoral program.

We would like to recall here a few interesting results obtained by Taras:

The first application of the generalized collective modes (GCM) to binary mixtures traces back to 1997, when Taras and collaborators employed [3] the parameter-free collective modes approach to investigate the collective excitation spectra of a gas mixture (HeNe). The study proceeded by comparing the theoretical prediction of the extended hydrodynamics, using different sets of variables, with the computer experiment. Remarkably, Taras and collaborators discovered that by incorporating an extended hydrodynamic set comprising seven dynamical variables, it was possible to successfully identify and characterize "fast sound" type modes in the gas mixture. Other sets were not capable of showing the existence of such a fast sound, a topic highly debated at the time. Through an in-depth analysis of the individual contributions of collective modes to the partial dynamical structure factors, he determined that these "fast sound" type excitations predominantly arise from the dynamics of the lighter helium particles within the mixture. This detailed examination not only shed light on the unique properties of the HeNe gas mixture but also **provided compelling evidence that the existence of fast sound modes is not limited to anomalous liquids such as water**. Instead, it indicated that this feature is a shared property among various disordered condensed matter systems.

A significant breakthrough in the field was the discovery that the parameter-free hydrodynamic theory, specifically the GCM approach, could successfully predict the existence of non-hydrodynamic transverse excitations and optics-like excitations in liquids [4–7]. This discovery opened up new perspectives on the behavior of liquids, revealing that they exhibit characteristics similar to elastic solids at high frequencies. In one pioneering paper [4], the transverse excitation of liquid cesium was thoroughly investigated. The study revealed that **shear waves begin to propagate above a specific wavevector** that is dependent on the system. **This finding fundamentally altered our understanding of liquids, demonstrating that they exhibit solid-like behavior at high frequencies**. In a subsequent paper [5–7], employing the GCM approach once again, transverse optics-like collective excitations were identified in two different models of binary liquids: a Lennard-Jones (LJ) mixture and a metallic alloy. It was demonstrated that these propagating modes arise from fluctuations in mass concentration, essentially representing mutual concentration waves. Notably, the analogy between these modes and optical phonon excitations in both high-temperature crystalline and amorphous systems is strikingly close, further highlighting the significance of these findings. These studies not only advanced our understanding of the dynamic behavior of liquids but also **underscored the versatility and effectiveness of the parameter-free GCM approach in predicting and characterizing complex collective excitations in diverse liquid systems**.

Taras studied an interesting problem on magnetically ordered structures on the surface of metals during his postdoctoral fellowship with Prof. Kleiman. The use of different variants of numerical methods led to contradictory results in the literature. In [8], Taras used the generalized gradient approximation with surface relaxation to study the magnetic properties of seven layers of V(001) film. The ferromagnetic ordering of surface atoms with an antiferromagnetic arrangement of atoms in the lower layers was found.

A comparison with other approaches was made. The experience of these rather complicated calculations was especially important for Taras's deeper understanding of first-principles modeling methods, in which he later became a recognized expert.

During his collaboration with Anthony Haymet [12–15], Taras made significant and groundbreaking contributions to the understanding of the physics of the water-ice interface, a complex problem that remains unsolved to this day. Employing classical molecular dynamics (MD) simulations as well as *ab initio* MD, Taras surpassed the results obtained for the SPC/E model with truncated long-range potentials. One notable achievement was accurately reproducing the density maximum of water, a critical characteristic of its behavior. Additionally, Taras successfully determined the melting temperature of ice through his two-phase simulations. Furthermore, he made crucial advancements in characterizing the local order parameter at the water-ice interface. By observing the change in tetrahedral environment across the interface, Taras was able to estimate the width of the basal ice-water interface, shedding light on the structural properties of this critical interface. Taras's work in this area represents a significant step forward in **our understanding of the intricate dynamics and properties of the water-ice interface, as well as specific behavior of solute ions at the water-ice interface**. His use of both classical and *ab initio* MD techniques, coupled with his ability to obtain essential thermodynamic quantities and characterize local order parameters, has contributed immensely to tackling the challenges associated with this complex phenomenon.

Taras made another significant and groundbreaking contribution that was published in Nature Physics [38]. His work revealed a remarkable discovery concerning the Widom line in supercritical fluids, **demonstrating that this line represents the transition between two distinct dynamical regimes: a liquid-like regime and a gas-like regime**. Conventionally, textbook definitions state that beyond the critical point, there is no physical observable that can distinguish between a liquid and a gas, resulting in a single fluid phase. However, certain thermophysical quantities exhibit maxima along a line extending from the critical point, known as the Widom line. Through a combination of inelastic X-ray scattering measurements and molecular dynamics simulations, Taras and his collaborators investigated the velocity of nanometric acoustic waves in supercritical fluid argon at high pressures. Their groundbreaking findings revealed a sharp transition upon crossing the Widom line, clearly demonstrating that the supercritical region can be divided into two distinct regions characterized by different dynamical regimes: a gas-like regime and a liquid-like regime. Although these regions are not connected by a first-order singularity, they exhibit similar characteristics to subcritical domains. This discovery not only challenged conventional understanding but also provided crucial insights into the behavior of hot dense fluids. Taras's work significantly advanced our understanding of the complex dynamics of supercritical fluids, which have immense importance in both fundamental and applied sciences. By shedding light on the existence of distinct dynamical regimes within the supercritical region, his findings have paved the way for deeper investigations and a more comprehensive understanding of these crucial systems.

The topic of the origin of organic materials on the Earth is an interdisciplinary one and is key to understanding such processes as oil formation, the origin of life, etc. A number of experiments have been performed in this area and several theories have been formulated that suggest certain favorable conditions for the relevant chemical reactions to occur, leading to the formation of hydrocarbons. The research conducted by Taras in collaboration with Anatoly Belonoshko [58] is quite original in this regard. They performed *ab initio* molecular dynamics simulations of the C-O-H-Fe system and found that such conditions exist at the core-mantle boundary (CMB). In particular, it was shown that the synthesis of complex organic molecules with C–C bonds is possible under conditions of reduced activity of oxygen. H_2O and CO_2 delivered to the CMB by subducting slabs provide a source for hydrogen and carbon. **The mixture of H_2O and CO_2 subjected to high pressure (130 GPa) and temperature (4000 to 4500 K) does not lead to synthesis of complex hydrocarbons. However, when Fe is added to the system, C-C bonds emerge. It means that oil might be a more abundant mineral than previously thought**.

The peculiarities of the atomic structure and spatial distribution of the charge density in a hydrogen fluid in the region of transition from molecular to atomic fluid at a temperature of 2500 K were determined [54] by *ab initio* simulations. It was analytically shown that the long-wave asymptotics of structural charge density factor for molecular hydrogen (low pressures) and metallic hydrogen (ultrahigh pressures) fluids should be proportional to the fourth power of the wavenumber $\sim k^4$. This was confirmed by computer simulations. However, in the region of the transition from molecular to atomic fluid, a sharp

change in the long-wave asymptotic coefficient arising from strong fluctuations in the electron density was found. This affects the proton shielding and, as a consequence, the contribution of the ionic component with a long-wavelength asymptotic $\sim k^2$ to the structural charge density factor in the transition region appears. This means that **in the transition region from molecular to atomic fluid there may exist not fully shielded ions**, which, in particular, is reflected in the peculiarities of the structure and dynamics of the hydrogen fluid in the transition region.

This Special issue of "Condensed Matter Physics" presents contributions from Taras Bryk's collaborators and friends, and covers a wide range of topics related to his research interests. The Guest Editors and the contributors of this Special issue, the Editorial Board of "Condensed Matter Physics", his numerous colleagues and friends would like to congratulate Taras Bryk, wish him Happy Birthday and to stay in good shape for long active years in science.

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Ihor Mryglod, Institute for Condensed Matter Physics, Lviv, Ukraine

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