

Obituary

In memoriam: Stefan Sokołowski



*Stefan Sokołowski at the Ulam Computer Simulations Workshop
(Lviv, June 21–24, 2017)*

It is our real pain to write this article, remembering years of friendship and scientific collaboration with Stefan Sokołowski, who passed away on the 24th of June 2024. He was a strong man in his faith and convictions, a kind and helpful friend, attentive and open-minded in discussions, creative, profound and sophisticated in understanding the flow of life and science. He left an unforgettable mark on our hearts and personal memories. His way of thinking left an imprint on students, young scientists and co-workers. We accompany all that with warm farewell applause as an appreciation of Stefan's way and effects throughout his life.

Stefan Sokołowski was born on January 18, 1951 in Bilgoraj in eastern Poland. After finishing primary and secondary education in Bilgoraj, he entered the Faculty of Chemistry of Maria Curie-Skłodowska University (UMCS) in Lublin in 1968. In 1973, he graduated from the faculty with an M.Sc. degree in chemistry. Next, he received a PhD grade in physical chemistry in 1977, after doctoral studies at the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw. His thesis, “Virial expansions of three-dimensional models for gas adsorption at solid surfaces”, was completed under the supervision of Prof. J. Stecki. In 1987, S. Sokołowski defended his habilitation dissertation entitled “Statistical description of gas adsorption at solid surfaces: two- and three-dimensional models of adsorption” at the Faculty of Mathematics, Physics and Chemistry, UMCS, Lublin, Poland. In 1997, he was awarded the title of Full Professor in Chemistry.

Despite almost purely chemical education, he extended his horizons to physics and mathematics by entering classical statistical mechanics of liquids and applications of mathematical numerical methods in this area of research. However, Stefan kept his affinity and preserved the admiration of experimental studies throughout his life.

During his scientific life, Stefan published over 500 articles in journals of very different profiles. His contributions range from the very top journals in physics and related areas, such as *Physical Review Letters*, *Physical Review A*, *B* and *E*, *Journal of Statistical Physics*, *Journal of Chemical Physics* and *Journal of Physical Chemistry*, and *Journal of Colloid and Interface Science*, to more specialized journals such as *Journal of Chromatography A*, *Acta Agrophysica*, and *Soil Science Society of America Journal*. His works all together received around six thousand citations in scientific literature. Chronologically, the first of them which still preserve the historical appeal to the origins of classical statistical mechanics were published in local media that may seem a bit exotic nowadays, namely *Annales Universitatis Mariae Curie-Skłodowska* and *Annales Societatis Chimica Polonorum*, in the mid of 1970s [1, 2].

Starting from the origins of his academic career till the end of his life, principal attraction of Stefan was in the study of fluid-solid interfaces. The systems of his interest on the one hand, involved models of purely academic impact but of profound importance for the construction of advanced theories for realistic fluid models. On the other hand, he liked to study problems directly related to experimental research.

Immediately after terminating his university education in 1974, Stefan, as one of the best students, received an offer and started a job as an assistant at the Faculty of Chemistry of the UMCS. He entered the Department of Theoretical Chemistry to teach and perform research in the area of adsorption of gases on heterogeneous surfaces under the supervision of Prof. W. Rudzinski. The years 1974–1976 were very productive for Stefan. Together with his tutor and co-workers, he published around twenty articles in highly prestigious journals. Within an ample problem of construction of the theory of adsorption of fluids in heterogeneous adsorbents, Stefan Sokołowski was focusing on applying Mayer-type virial expansions to describe adsorption and to use gas chromatographic data for the characterization of heterogeneous adsorbents. At this stage, it is worth to pay tribute to the leadership of Prof. Rudzinski in this project and fruitful collaboration of Stefan with M. Jaroniec. They kept friendship for many subsequent years.

In the desire to get a deeper knowledge of the methods of statistical mechanics of fluids and its application to interfacial phenomena, S. Sokołowski, in parallel to his permanent job, has inscribed to doctoral studies at the Institute of Physical Chemistry belonging to the Polish Academy of Sciences, under the supervision of Prof. J. Stecki. One can imagine how much effort was necessary to face and successfully fulfil all necessary tasks. Stefan received the PhD grade in 1977, as already mentioned above.

The contents of the thesis are reflected in six publications of S. Sokołowski and J. Stecki. It is worth mentioning the contents of [3], in which the validity of the two-dimensional approximation to the description of gas adsorption on solids was explored for Lennard-Jones and other fluid models. This type of development was re-invented to describe the adsorption of associating fluids on solid surfaces three decades later in several works within the two-dimensional statistical associating fluid theory (SAFT-2D). Conceptually novel elements, in comparison to the virial expansion for the density profile [4], were proposed by Sokołowski in [5, 6]. Namely, the first- and second-order integral equations for a hard-sphere fluid in contact with a hard wall were solved to explore the inhomogeneous pair distribution function besides the fluid density profile.

In 1983, S. Sokołowski succeeded in obtaining a one-year postdoctoral position at Penn State University in the laboratory of Prof. W. A. Steele. There, for the first time in his scientific growth, he applied the local density functional approach as a natural extension of the previously used integral equations methodology to study the adsorption of simple fluids on solids. Moreover, the method was used to explore the freezing of a hard sphere fluid under the influence of the external field [7]. Another novel element for Stefan was applying molecular dynamics simulations for adsorption phenomena [8]. Additionally, Stefan gained skills in describing crystalline solid surfaces.

In 1988, S. Sokołowski got the Alexander von Humboldt Fellowship at the Institut für Thermo- und Fluiddynamic of Ruhr Universität in Bochum, to collaborate with Prof. Johan Fischer. During this period, Stefan mastered his skills in the application of non-local density functional techniques, explored the combination of density functionals with the Born-Green-Yvon integral equation for the density profile and made progress in the application of molecular dynamics computer simulations to study the adsorption of binary mixtures in slit-like pores [9–11].

At this moment of his life, Stefan became a well-established scientist with his own ideas, with vast and profound knowledge of analytic, numerical and simulation methods within the theory now commonly referred to as soft condensed matter, with special emphasis on interfacial phenomena. Also, he became known to the liquid state theoretical community on an international scale. Consequently, Stefan felt free to undertake challenging projects according to his taste. Thus, without long meditation, he accepted the invitation of Hans Herrmann for a visiting professorship (1990–1991) in Forschungszentrum in Jülich. The freshly launched project on the transport of granular materials was developed with H. Herrmann and J. Gallas. One of the outcomes of the project involved molecular dynamics simulation of granular media [12, 13]. Reference [12] is the most cited contribution of Stefan.

On the temporal axis, Stefan spent his last long-term stay out of Poland in 1994–1995, attending the invitation of Prof. Douglas Henderson to work together at Autonomous Metropolitan University in Mexico City. During his stay as a visiting professor, Stefan undertook a study of topics that were novel to him. Namely, in this laboratory, Sokołowski considered the problem of electric double layer by using density functional approaches, integral equations and Monte Carlo computer simulations. These theoretical techniques were applied at the level of primitive and solvent primitive models of electrolyte solutions. A bunch of influential results were published within this project [14–17]. Moreover, Stefan addressed several problems related to the description of colloid solutions and model membranes. In addition, he proposed a novel energy route within the density functional approach to capture liquid-vapour phase behaviour of the restricted primitive model electrolyte under confinement [18].

For many years, Stefan was involved in the studies of models with very different ranges of interactions. We do not mean the models of interaction between particles but rather the interaction between Stefan and the scientific medium around him. The classical model of nearest-neighbour interaction should be the one between Stefan Sokołowski and Andrzej Patrykiewicz. They knew each other from the student times and started collaborating in 1983, e.g., [19]. In what follows, they worked together on very different short and long-term projects. One of their principal common research areas was the application of Monte Carlo simulation methods to investigate the superstructure formation and phase behaviour of adsorbed films formed on crystalline surfaces and in nanoscopic slit-like pores with crystalline walls. A rather comprehensive description of their work and achievements reached in collaboration with Prof. Kurt Binder can be found in a highly cited review paper [20]. On the other hand, an extended treatise of theoretical methodology for inhomogeneous fluids containing strong pedagogical fundamentals, together with advanced original findings, was elaborated in [21].

Another “binding-type” nearest-neighbour model of scientific collaboration of Stefan during many years was with his wife, Zofia Sokołowska, Professor at the Institute of Agrophysics of Polish Academy of Science, whose principal research line is physico-chemical properties of soils. For many years, they investigated the adsorption on soils by combining experimental results and theoretical elements, e.g., from the theory of microporous disordered media, [22–24]. However, one of the valuable contributions was in developing a new approach to analyse the mass fractal dimension of soils for environmental research [25, 26].

The models of next-to-nearest-neighbours scientific interaction refer to Hungary and Ukraine. In 2007–2009, Stefan actively collaborated with Laszlo Pusztai (Wigner Research Center of Physics at Budapest). They were interested in a wide set of systems, from hard sphere fluid models to realistic water models [27], and various phenomena ranging from adsorption to the microscopic structure of solutions in bulk and under confinement [28], as well as freezing and formation of the glass phase (see, e.g., [29]). Methodological issues of this collaboration involved common molecular dynamics, reverse Monte Carlo modelling and the numerical solution of replica Ornstein-Zernike integral equations.

Stefan had long-lasting strong links with researchers from the Institute for Condensed Matter Physics (ICMP) of the National Academy of Sciences of Ukraine in Lviv. In particular, he collaborated with Yu. Kalyuzhnyi on inhomogeneous associating fluids [30, 31], with J. Ilnytskyi [32, 33] on the problems of fluids adsorption in disordered porous media. The latter project in the following years was extended to optimize the computer design of nanoporous systems with the desired properties and to search for novel materials with applications in chromatography. A range of ideas by Sokołowski found their realization in the studies of the formation of complex structures in the binary mixture confined within a pore with pattern-decorated walls by dissipative particle dynamics simulations with J. Ilnytskyi and T. Pat-sahan [34, 35]. Other studies within the project concentrated on self-assembly of pattern-functionalized

nanoparticles into gel-like structures by coarse-grained molecular dynamics. Common research with A. Kovalenko, Yu. Duda, S. Hlushak, and T. Bryk (all of them from ICMP) resulted in a bunch of publications concerned with specific theoretical problems of the microscopic structure and thermodynamics of fluids and fluid mixtures under the confinement of pores. One of the long-term collaborations of Stefan was with A. Trokhymchuk. They started to work together in 1995 in Mexico [36], and their last common paper [37] was published in 2011. This collaboration focused on inhomogeneous associating fluids is marked by a variety of methodological tools, e.g., from the singlet associative replica Ornstein-Zernike integral equations [36] to the application of Born-Green-Yvon equation for the density profile [38], Monte-Carlo computer simulations [39], to the pair level theory of non-uniform associating fluid [40]. In this latter work, the Wertheim theory for the bulk association was combined, apparently for the first time, with the pair level theory for inhomogeneous fluids.

Stefan made an essential contribution to the development of theoretical chemistry at UMCS in Lublin (Poland). He was eagerly and permanently working and publishing with his close circle, M. Borówko, W. Rżysko, P. Bryk, and T. Staszewski. He was a supervisor of the PhD theses of his students, G. Chmiel, P. Bryk, J. Reszko-Zygmund, K. Bucior. He served the scientific community as a permanent reviewer of works in many top journals, such as the Journal of Chemical Physics, Journal of Physical Chemistry, Physical Chemistry Chemical Physics, and Physical Review, as an external reviewer of several projects and many PhD theses, and as a member of specialized scientific councils. He was the coordinator of the project “Statistical Thermodynamics and Computer Simulations of Complex Molecules in Bulk and at Surfaces” (STCSCMBS), which was supported by the EU within the 7th framework programme.

Prof. Sokołowski was a very experienced lecturer and teacher. For many years, he taught courses on statistical thermodynamics, surface phenomena, phase transitions, computer simulation methods (Monte Carlo and molecular dynamics) and programming. He was skilled in attracting students into research in chemical physics. Stefan Sokołowski received several distinctions and awards, namely the Humboldt Fellowship and Doctor Honoris Causa of the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine (November 26, 2019) for extraordinary scientific achievements in collaborative research. For many years, he served as editor of the Condensed Matter Physics journal published by ICMP.

To provide a summarizing insight, Stefan Sokołowski, during his life, contributed to the study of a variety of systems, namely of simple fluids and associating fluids, fluid mixtures, electrolyte solutions, fluids of chains, Janus particles, granular media, micro- and mesoporous media, soils. He explored several phenomena, such as fluid-solid and liquid-liquid interfaces, adsorption on solids, crystalline surfaces and chemically modified surfaces, surface phase behaviour and electric properties at interfaces. He made valuable contributions using and extending different methods of liquid state theory, namely of virial expansions for the density profile and adsorption isotherms, integral equations, scaled particle approach, density functional techniques, Monte Carlo and molecular dynamics simulations, and dissipative particle dynamics. Undoubtedly, the scientific community has benefitted from his work and will continue to use his results in future developments.

Andrzej Patrykiewicz, personal: My acquaintance with Stefan began in 1976 when I graduated from the University of Lublin. Stefan was already an assistant at the Department of Theoretical Chemistry in our Faculty of Mathematics, Physics and Chemistry at UMCS. From the beginning, he impressed me with his knowledge, openness and ability to find interesting research problems. I have had the opportunity to cooperate with him for over forty years, and I could always count on his help in solving various problems. He had a unique ability to find answers to difficult questions. In the years of our “scientific youth”, we spent entire days, and often even nights, making questions, trying to find solutions, and writing countless programs for calculations using Monte Carlo methods and density functional theory. In those years (1980–1985), there was no Internet, only an internal academic network (called QQ) that required working at the only available monitor connected to the computer centre of our Faculty.

In the following years, our close cooperation brought fruits in many ways. We had several joint projects involving many prominent scientists from many countries (Kurt Binder, Carlos Vega, Johann Fisher, Siegfried Dietrich, Martin Schön, among others). I must emphasize that Stefan was very modest and did not care about honours. He never tried to show dominance and always supported his younger colleagues.

I would also like to stress that Stefan was a great colleague. I will always remember our joint visits

to many research centres in Europe (Mainz, Prague, Madrid, Lviv) and Mexico, where we worked with Orest Pizio. Although the primary purpose of these trips was scientific cooperation, there was also a time for feasts and learning about local customs, cuisine, and wines. Even over wine, our discussions usually evolved to new projects. I cannot express my sadness at his passing, and I will always miss the discussions (often very heated) and the opportunity to meet him at the Institute.

This shouldn't have happened, at least not yet.

Carlos Vega, personal: I met Stefan for the first time in Bochum in the spring of 1989. At that time, I was a PhD student, and I was impressed by the fact that a young professor from Poland was leaving the lab even later than I did. We became friends at that time, and we talked about science, life and almost everything. I still remember him taking a train to Poland in June 1989 to vote for the first time after many decades. His compromise with democracy and with Poland was first. He brought a bottle of "special vodka" from Poland, and we celebrated together the return of democracy to Poland. After that, we met many times at the Liblice conference organized by Ivo Nezbeda, and even more when Poland joined the European Union, and he was the coordinator of an EU program. With this program, several persons from our group in Madrid (Jose Luis F. Abascal, Luis Gonzalez MacDowell) visited Lublin (Poland) for several months. Also several persons from Lublin visited Madrid (Stefan himself, Andrzej Patrykiewicz, Małgorzata Borówko, Pawel Bryk). We also organized a symposium in Madrid, and I still remember Stefan visiting Toledo and suffering with the hills of the city. I must say that the time I spent in Lublin (two months) was one of the best summers of my life. With my wife and my two kids, we spent two months in Lublin, and besides doing good science we had very good memories. We often attended the parties organized in Stefan's house with his family before returning home with a taxi. Stefan was quite generous with his wisdom (it was always a pleasure to chat with him about science). Several papers were published from this collaboration Lublin-Madrid, and I am particularly proud of my "Lublin" papers on the free surface of ice in collaboration with Andrzej, which were possible thanks to the invitation of Stefan to visit Poland.

On the professional side, Stefan was a solid scientist doing serious research, able to write a program about almost everything (theory, simulation), and with a deep knowledge of statistical mechanics. To my mind, the work of Stefan was always solid, robust and interesting. He never aimed to follow fashion but rather followed his curiosity. We met many times in different places (including Lviv in Ukraine, Mexico city). I still have on my table a cloth that Orest and Stefan gave me as a present when we visited Teotihuacan in Mexico on an unforgettable day. Stefan was the kind of person that made this life nicer. He was a good scientist from the first day to the last one. I learned many things from him in the early days of my career when we worked together on Saturdays at the University of Bochum. Hard work in science is first, and he was an example to follow. Also, on the personal side, he was a very nice person, a good teacher, a good researcher, a good father and a good friend. I will miss him and the many moments at which we enjoyed science and life together since 35 years ago.

László Pusztai, personal: I met Stefan several times between 2006 and 2010 at UNAM, Mexico City, where we used to visit Orest Pizio at the Instituto de Química. I was immediately impressed by his gentle manners, by which he was able to convey his vast knowledge over various subjects. The three of us had good times spent with discussions of science, as well as life in general. I felt overwhelmed and privileged when Stefan invited me to spend a couple of months at his university with him in Lublin, as part of an EU project he participated in.

I spent two unforgettable months in Lublin during the first half of 2008. We spent quite some time discussing issues related to interatomic potentials in water and aqueous solutions of rubidium bromide. He patiently and attentively listened to my attempts to describe diffraction experiments and reverse Monte Carlo modelling — topics he had not previously dealt with. Out of this mixture of concepts, a publication in *J. Chem. Phys.* has emerged.

It was always a pleasure to meet Stefan at various occasions since then. Although his scientific activities turned more towards purely theoretical issues, I profited enormously from discussions with him. His passing is a loss for all of us who were fortunate enough to know him.

Jaroslav Ilnytskyi, personal: I got acquainted with Stefan in 1998, having a one-week scientific stay in Lublin organized by Orest Pizio. It was upon returning from the workshop on liquid crystals in Erice, Italy, and ended up straightaway with two papers of a much higher calibre than I had ever published before. Besides that, I learned from Stefan that: a set of accessible computers were called after the notes

of a musical gamut, one should never use general words for passwords, what Web of Science is, as well as understanding some tricks of the trade in computer simulations.

When doing collaboration research, Stefan was not only distinguished by his vast knowledge of methods and approaches, both theoretical and computer simulation ones, but also by his healthy scepticism and irony. This steered collaboration work away from being a pathetic routine into some realms that are more associated with art. No wonder he had a nice collection of paintings. He regularly listened to the Polish cultural radio station “Radio dwójka” and had a deep knowledge of classical music. He had an exhaustive experience in house construction technologies. Never forget his kindness towards pets: at some stage, his family took care of about five cats. On top of that, he always had a deep involvement in gardening.

Stefan was an excellent teacher. There was no pressure, not a glimpse of a wish to push his personal point of view. Instead, he always tried to convince, patiently waiting for the younger colleague to find his or her own way, even if the things were too obvious. Stefan gladly exchanged his views and experience if you really wish to do so and are ready to digest this information. It was for sure for me that Stefan always put good friendly human relations above dry and painful constatation that someone was wrong, and if so he found a way to relay this information in the least harmful way.

I spent in total about a year and a half in Lublin, by monthly exchange visits within the EC FP7 project. Stefan was very enthusiastic and put a lot of effort into writing and shaping up our application. We published a dozen papers during this lovely time. The atmosphere in the Department was truly free and informal, and it was always a great pleasure to stay there. No one rushes anywhere. You can take your time to think about things. As Ernst Rutherford once remarked: “If you work in the lab all the time: when do you think?”. People in the Department really had this culture of scientific thinking and discussion. Besides thinking, you can also play the flute, what I did, enjoying the unforgettable acoustics of the computer class.

These are really very deep and sad feelings about Stefan, both a scientist and a charismatic person, leaving this world, and there are always regrets on my side for not being active enough in collaboration or not learning from him as much as I really ought to. Rest in peace, our dear colleague and friend.

Orest Pizio, personal: Bright and sharp mind, extraordinary technical skills, extremely disciplined, unlimited desire to learn new things. His appealing motto “This sounds interesting, let us write a program now” is a good guide for younger generations, as it was for us. There had been three decades of common work (since 1994 in Mexico), three decades of the most productive and most fruitful scientific life. Three decades of true friendship. So many words can be said, but I cannot find words to express my loss.

Taras Patsahan, personal: I remember that Stefan always enjoyed visiting Lviv, where he could discuss scientific problems and have a good time with his Ukrainian friends. He liked to go to the Lviv Cathedral each Sunday during his stay in Lviv. Unfortunately, Stefan’s last visit to Lviv was interrupted due to COVID-19 pandemic restrictions. In 2012 and 2023, I spent a couple of months in Lublin, working closely with Stefan on the FP7 project in his lab. There, I learned a lot and gained new, useful scientific experience. We worked together on computer simulations of polymer brushes in contact with different solvents using molecular and dissipative particle dynamics. I have unforgettable memories from my time in Lublin. I am proud to have had an opportunity to interact with Stefan. He was a scientist and a person worth following and setting as an example for others. We will miss him very much.

Andrij Trokhymchuk, personal: I met Stefan Sokołowski for the first time in Mexico City in August 1994. Due to Stefan’s presence around, this year and half of 1995 were the most remarkable in my professional growth. Stefan was my guide to learn the Monte Carlo simulation method. After 2008 I visited Stefan many times in Lublin. In turn, Stefan loved to come to Lviv. He actively participated practically in all international meetings on the statistical physics of liquids and soft matter that took place in Lviv. The last one in this row was the Ulam computer simulation workshop in 2017 (<https://icmp.lviv.ua/ucsw2017/index.html>). The last time we met with Stefan was in September 2023 when I spent a night at his lovely home in Lublin travelling from Lviv to Ljubljana. Stefan was full of energy and scientific plans for the nearest future. The same words about Stefan I heard again from his colleagues and students at the funeral ceremony in Lublin on August 3rd. Rest in peace, my dear Stefan, dear Professor Stefan Sokołowski.

Rest in peace, our dear friend and colleague...

*Orest Pizio (Institute of Chemistry, National Autonomous University of Mexico, Mexico),
Andrzej Patrykiewicz (Maria Curie-Skłodowska University),
Carlos Vega (Universidad Complutense de Madrid, Spain),
Laszlo Pusztai (Wigner Research Center for Physics, Hungary),
Jaroslav Il'nytskyi (Institute for Condensed Matter Physics, Ukraine),
Taras Patsahan (Institute for Condensed Matter Physics, Ukraine),
Andrij Trokhymchuk (Institute for Condensed Matter Physics, Ukraine).*

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