In Memory

Professor Marek Cieplak

(1950–2021)

Marek Cieplak, born December 8, 1950, passed away on December 31, 2021. He was a Professor of Physics, a lecturer of summer courses in physics at Rutgers University and Johns Hopkins University in the USA, a member of the Scientific Council of the Institute of Physics of the Polish Academy of Sciences (PAS), initiator of biophysical topics at the Institute of Physics PAS, founder and head of the Laboratory of Biological Physics, spiritus movens of the series of international scientific conferences *"Biomolecules and Nanostructures"*, **member of scientific societies and editorial boards of scientific journals such as** *Journal of Physics: Condensed Matter* **and** *Acta Physica Polonica A*.

Figure 1: The commemorated Marek. Photo taken from the family resources with permission.

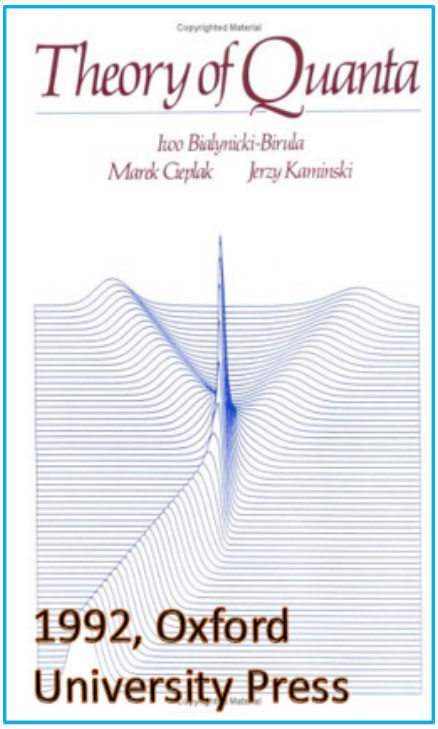

Figure 2: (Top panel) Marta Gieburowska (Cieplak) and Marek Cieplak, students of the Faculty of Physics, University of Warsaw in the Large Experimental Hall (SDD). (Bottom panel) Marek — as a student — got involved in helping Professor Białynicki-Birula to prepare notes for his lecture on quantum mechanics. These notes eventually evolved into a book, which Marek co-authored with Professor Białynicki-Birula and Professor Jerzy Kamiński, many years later. Photos taken from the family resources with permission.

This issue collects several articles that aim to symbolically commemorate Marek Cieplak, not only because of his profession. All articles went through the peer review process, and the authors and reviewers deserve thanks.

The unusual and unique feature of this issue is not only its scientific content, but also the inclusion of several personal recollections. Below are short texts about Marek, as he is remembered by colleagues, former PhD students (now full-fledged scientists) and his friends. The editors appreciate their presence and sharing! It is worth reading these personal recollections because they outline the broader profile of Marek, his human qualities for which he was appreciated.

The editors

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Marek Cieplak was a man full of passion — both in physics and beyond. You could feel the strength of his personality already as you approached his office, which stood out against the gray and somewhat colorless corridors of the Institute of Physics of the Polish Academy of Sciences — the door was always open, and inside it was filled with flowers, paintings, posters, and figurines. Once you stepped in, Marek would tear himself away from his inseparable computer and bombard you with a vast number of scientific ideas, intertwined with the latest cultural curiosities, books he had read, movies he had seen, or travels, which he was passionate about. Marek's research was just as eclectic — from work on spin glasses, to the analysis of river networks, optimal paths in disordered systems, fluid invasion into the porous media, and the microscopic origins of friction. In the last 25 years, his main focus has been biological physics, in particular numerical models of protein folding and unfolding, interpretation of genetic microarray data or knots and entanglements in biomolecules. We collaborated on many of these subjects, publishing 15 papers together.

I will miss his energy, passion, and drive to keep moving forward. I am grateful for the time we shared and for the inspiration he brought to our work.

Piotr Szymczak

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Professor Marek Cieplak, as we all know, was an extraordinary character, a person who always had his own opinion, always had substantive arguments and was able to defend them to the end. This was also Marek's whole life... and this state of mind was contagious to others — to me certainly. I had the pleasure of being a doctoral student of Professor Cieplak. Marek's knowledge and behavior had a huge impact on my scientific career and on my decision to follow this path. Marek was 110% committed to every doctorate, and he demanded the same! He was at work every day, he came every day to talk about both science and life. His room at the Institute of Physics was full of flowers, paintings and souvenirs brought from his travels around the world, as well as two, sports items: a tennis racket and a bicycle. Marek cycled to work whenever he could. His wife and daughters painted the paintings. This room looked like a real museum — it always encouraged me, even when Marek asked rhetorically: "Why don't computers count when it's cold outside, or why don't I have the conscience to freeze them like that?" He did it jokingly, but you could still feel a shiver of fear. Yes, he definitely made sure that the learning progressed and that every moment was well-planned and used. I remember well that before I left for trekking in the Himalayas, he

made sure that I had a copy of my data and that I had planned the calculations appropriately so that the computers would not "freeze" during my 3-week trip. On the other hand, after returning I saw how happy he was, not only that the data had been calculated, but that I had returned in one piece. Marek was caring; he was hot-tempered, but he always meant well and strived for objective truth.

From a scientific point of view, I think it should be strongly emphasized that the topic of non-trivial topology in proteins, which I continue to develop (as do a lot of scientists around the world), was born by accident, but this accident was created by Marek. One day in 2006, just before the holidays, Marek came up with the idea to determine the free energy landscape of proteins from the point of view of mechanical resistance. This idea probably resulted from the fact that at that time single-molecule optical tweezers, which trapped micron-sized silica beads (of diameter range of 0.2–5 m) to exert forces on the system of interest, achieved very high precision in measurements, showing that titin (the protein that makes up our muscles) has a mechanical resistance of about 210 pN. On the other hand, the mechanical resistance of the calcium-binding C2A protein has been found to be much weaker, i.e., the peak force is only of order 60 pN. Marek's goal was to learn the limits of the mechanical strength of proteins and to understand whether this feature correlates with the biological function or perhaps the spatial structure of proteins.

The idea was brilliant (more on that below), but what was worse, Marek wanted to do it in his own style, i.e., as best as possible. That meant writing a program to stretch (possibly in many direction) all known protein structures deposited in the Protein Structure Database in 2006. At that time, there were over 50000 structures. This idea was in the style of current big data, although such an approach was not yet used at that time. Marek always did things ahead of his time. So the man had to bite the bullet and rise to the challenge. The idea was also very successful from the point of view of the so-called Go-like model, which Marek created with his PhD student (Professor T.X. Hoang). In the Go-type model that Marek used, two factors played a major role: native contacts (defined based on the geometry of the protein in its native state) and the spatial structure of the protein (alpha-helices, beta hairpins). Therefore, the model performed is ideal for studying mechanical properties, starting from the native structure of the protein. After 6 months of research, it was possible to find proteins whose resistance force was over 1000 pN. It turned out that among these proteins there were proteins with non-trivial topology knotted proteins. Our first reaction was that this must be a mistake — none of us knew or expected knots in the proteins to exist.

There are proteins that show such high mechanical resistance. However, proteins with non-trivial topology show lower resistance, and in such a case the observed force comes from the knot tying, but thanks to that, we were able to find them. Today, the study of non-trivial topologies in proteins has become a separate, dynamic research field at the intersection of biophysics, biochemistry, and mathematics. Marek's works are among the best cited on this topic, and a collection of his works forms the basis of a review entitled "Topology in soft and biological matter" published this year in *Physics Reports* **1075**, 1 (2024).

Joanna Sułkowska

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The outstanding role that Professor Marek Cieplak played in theoretical physics, condensed matter physics, and biological physics is beyond dispute. However, I personally believe, and I would like to emphasize, that all these achievements were possible thanks to his exceptional personality.

Marek was a visionary, an inspirer and a titan of hard work, constantly seeking new inspirations with tireless energy, determination and scientific passion, along with many humanistic interests. He was always on the lookout for scientific developments, driven by the energy and determination to bring ideas to fruition. The word that best describes Marek is "passion" and he embodied this spirit, as lively and tireless as a great fire.

Marek had one mantra that he often repeated and consistently implemented: "Don't give up without a fight!" This was his Golden Thought. He always took the bull by the horns. I remember him as a person for whom nothing was too difficult to at least try. That is why he had a remarkable ability to motivate colleagues to push beyond their limits.

He was the initiator of introducing biological physics at the Institute of Physics of the Polish Academy of Sciences. Fueled by Marek's enthusiasm and determination, in 2004 we began our activity as a small Biological Physics Group SL-1.5. Our first challenge was to secure funding and set up experimental laboratories. We acquired space in an old transformer station and storage area at our Institute, where I started building laboratories equipped with the essentials to commence experimental work, with great support from Marek. Over time, many people joined the group, new topics emerged, including nanotechnology, and our group was upgraded to the Laboratory of Biological Physics SL-4. However, we still needed significant changes and investments, as our initial setup was quite basic.

I must emphasize that Marek's tireless enthusiasm for taking on risky initiatives was one of the strongest motivational impulses I have ever experienced. I am certain that the energy derived from daily interactions with Marek was vital in undertaking such ambitious projects. It ultimately led me to establish a consortium to create seventeen new laboratories in Poland, including our own microspectroscopy laboratory and a second computer cluster for Marek's group within the POIG ERDF NanoFun Project.

One of the most significant contributions by Marek to sharing high-level science with society is the "Biomolecules and Nanostructures" (BioNano) conference series. Marek envisioned this event as an opportunity for scientific friends to meet and discuss topics in an informal atmosphere. It resembled a group retreat, yet extended to around one hundred participants in a secluded area, far from large cities. The great success of these conferences stemmed from the fact that Marek's friends and collaborators from all over the world came together to meet him in person. He deeply valued his scientific friendships.

Over the years, we have transformed the meeting from an extended group retreat called the "Workshop on Structure and Function of Biomolecules" (2004, 2006) into an international scientific conference series "Biomolecules and Nanostructures" (2011, 2013, 2015, 2017, 2019), while maintaining the informal character of the meetings. The broader framework of the BioNano conferences also aligned with Marek's further involvement in nanobiotechnology studies. The venues changed, always close to nature and often in spartan accommodation, but the priority was still on the quality of the lectures and scientific discussions, fostering connections and collaboration among attendees rather than focusing on comfort. The conference grew, and Marek remained close to and engaged with the participants.

The great added value of the BioNano conferences lay in crossing barriers between the exact and natural sciences and the humanities — this was interdisciplinarity and multidisciplinarity in the best sense of the word. The opening lectures led the audience from linguistic methodology to molecular biology and from fundamental physics to physiology and evolution. This was made possible because, in addition to his great commitment to scientific matters, Marek moved us with his humanistic sensitivity. He often noticed little things that helped us feel more integrated with the world.

Marek was also always accompanied by his family. It was truly remarkable that despite his immense commitment to his professional career, he always maintained close ties with his loved ones.

Professor Marek Cieplak exemplified a rare combination of great ambition and versatile competencies, constantly seeking new inspirations. I remember him sitting in his armchair, going through the latest issues of *Nature* or *Science*, selecting topics that were new to him and to which he could apply the methods he had developed in order to join a new field.

Marek was always "on the ball", catching everything and hitting the mark. He will remain in my deepest memories.

Anna Niedźwiecka