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The interview with the author of the PhD thesis: "Collisions of simple molecules and atoms in fundamental studies"

Your work concerns a very specialized topic. Could you briefly explain what your research is about?

My work focuses on collisions between simple molecules and atoms – processes that are constantly present all around us, even though we usually don't pay attention to them. At room temperature, nitrogen and oxygen molecules in the air move at astonishing speeds, colliding billions of times per second. We don't usually think about it, but these processes are incredibly important – for example, in Earth's atmosphere, in outer space, or in precise laboratory experiments.

In my work, I examined such collisions at the level of individual molecules, performing precise calculations using quantum mechanics. I focused on two main goals: first, to generate accurate data that can support, for example, the monitoring of greenhouse gases and pollutants in Earth's atmosphere; and second, to explore several more fundamental questions in quantum theory – such as how to interpret collisions of indistinguishable molecules in the presence of electromagnetic field, or how weak interactions between nuclei influence molecular collisions.

In what ways might the findings of your research be applied within the field of astrophysics?

In two ways. First – in the interstellar medium, where stars are born, the conditions are extreme: there are very few molecules, and both temperature and pressure are extremely low. To understand what's happening there, we need to know precisely how individual molecules collide and how they interact with electromagnetic field. Without this knowledge, it's easy to misinterpret observations made, for example, by the James Webb Space Telescope. Second – my research helps analyze the atmospheres of planets and exoplanets. In those environments, there are vast numbers of molecules constantly colliding, which distorts the signals we observe. Thanks to the accurate data provided in my thesis, these observations can be better "decoded": we can determine the chemical composition of the atmosphere, physical conditions, and even chemical processes or, to some extent, the planet's history.

To what extent did the resources provided by Cyfronet support the computational part of your dissertation?

Although the underlying theory is encapsulated in a single-line equation, solving it requires substantial computational power. In research on greenhouse gases, for example, we aim to determine the concentration of specific molecules with a precision better than one part in a thousand. That means millions of hours of CPU time and advanced software for solving the Schrödinger equation, which we develop in our research group. Thanks to the resources of Cyfronet, I was able to carry out such large-scale calculations, studying molecules that lie at the edge of what is considered feasible in this kind of research. In their absence, my research would have been restricted to the simplest systems with minimal practical relevance.

Which phase of your research turned out to be the most demanding?

The most technically demanding part was, of course, the quantum scattering calculations – it's a highly complex process. But once the program, scripts, and computational strategy are in place, running the calculations themselves is not particularly challenging.

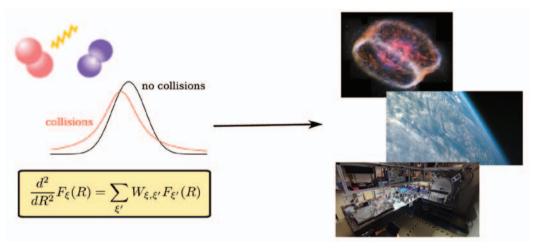
What brought the most challenges (and joy!) was solving the physical problems themselves. Finding the best approach – sometimes an entirely new path – was the most intellectually rewarding part. And the difficulties I treated more like puzzles that simply needed to be solved.

What mindset helped you get through the more difficult moments in your research work, and what advice would you give to young researchers who are struggling at the beginning of their journey?

In research work, it's impossible to avoid moments when you get stuck – something doesn't work, the code crashes, or the theory produces absurd results. It's frustrating. That's why collaboration is the key – talking to other researchers, even those outside your field, often brings new ideas.

It's also good to have a break – a smaller project, a hobby, sports, or music. The brain needs different kinds of stimulation to work effectively.

To young researchers, I would give one piece of advice: start as early as possible. The sooner you get involved in real research work, the more you'll gain – in knowledge and in confidence.



**Molecular collisions affect how they interact with light.** They cause broadening and shifting of spectral lines (see the two curves on the left side). Describing these effects requires complex quantum calculations (bottom left formula). Such studies are crucial for:

- **interpreting astrophysical observations** (top right image: NGC 1514 nebula, James Webb Space Telescope, www.webbtelescope.org)
- Earth's atmosphere research (center right image, NASA EarthKAM, www.images.nasa.gov)
- high-precision molecular spectroscopy used for testing quantum theory (bottom right image, cryogenic molecular spectroscopy lab at KL FAMO, Toruń).