



Bogdan Andrei Stoian

Computational Chemist · MSc Chemistry student

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Profile

Computational chemist studying how phosphaaalkenyl tetrylene ligands bind to transition metals, using DFT in Gaussian. I build structures by hand, set up batch calculations with scripts and write Python tools that extract results from large output files. Open to roles in computational chemistry, R&D, nanotechnology, scientific data and automation.

Research

Master's Researcher, Computational Chemistry

Oct 2025 – present

Babeş-Bolyai University, Cluj-Napoca

- DFT study (PBE0/def2-TZVP, Gaussian) of mono- and bis(phosphaaalkenyl)tetrylenes (E = Si, Ge, Sn; D = NHC, Et₂O) as capping ligands for gold nanostructures.
- Modelled how the ligands coordinate to group 11, 10 and 8 metals (Au, Pt, Fe) through P, through E, or both.
- Build structures by hand, then use scripts to swap elements and set up batch calculations; every input checked by hand.
- Python scripts that extract energies, stability constants and other results from output files with millions of characters.
- Run and monitor jobs on a remote Linux computing server; check structures in GaussView.

Oral presentation, "Students for Students"

22–25 Apr 2026

International conference, Cluj-Napoca

- Talk: *"Rational design of metal complexes stabilized by mono- and bis(phosphaaalkenyl)tetrylenes"*.
- Communicated results in English to an interdisciplinary student audience.
- Took part in scientific discussions and networking with international peers.

Education

MSc Chemistry

EQF 7

Oct 2025 – present

Babeş-Bolyai University, Cluj-Napoca

BSc Chemistry

EQF 6

Oct 2022 – Jul 2025

Babeş-Bolyai University, Cluj-Napoca

Knowledge

- Core concepts across inorganic, analytical, organic, physical and biochemistry
- Designing, running and supervising chemical experiments
- Analysing and characterising compounds and interpreting the results
- Operating laboratory equipment and instruments

Skills

- Qualitative and quantitative analysis of chemical processes
- Choosing physicochemical parameters, separation and purification methods
- Determining physicochemical and structural properties
- Quality control, risk assessment and safe handling of chemicals and waste

Responsibility & autonomy

- Working effectively in teams of specialists
- Respecting procedures, operating parameters and deadlines
- Applying health, safety and environmental regulations
- Working independently

Volunteering

- Helped organise and coordinate chemistry outreach events and experiment demonstration stands.
- Presented and explained experiments to children, high school students and the public.
- Ensured safe handling of chemicals and lab materials during demonstrations.
- Worked with other volunteers and academic staff on materials and event logistics.

Volunteer, Uniunea Studenților din România (USR)

Oct 2022 – present

- Volunteered at two editions of the Forum of Romanian Students Everywhere (now FTRP).
- Completed USR trainings in teamwork, leadership and project writing.

Skills

Computational chemistry

DFT

Gaussian

GaussView

Quantum chemistry

Coordination chemistry

Organometallic chemistry

Nanotechnology

Code & automation

Python

Process automation

Scientific data analysis

Generative AI tools

Linux (basic)

Lab training

NMR

X-ray crystallography

IR spectroscopy

Schlenk line

Glovebox

People & tools

Teamwork

Leadership

Proposal writing

Science communication

Presenting

Organisation & planning

Critical thinking

Analytical skills

Excel

Word

PowerPoint

Digital skills

Information and data literacy

●●●●●●

Advanced · 6/6

Communication and collaboration

●●●●●●

Advanced · 5/6

Digital content creation

●●●●●●

Intermediate · 4/6

Safety

●●●●●●

Advanced · 6/6

Problem solving

●●●●●●

Advanced · 5/6

Self-assessment based on the EU Digital Competence Framework (DigComp 2.1).

Languages

Romanian, native

Language	Listening	Reading	Spoken production	Spoken interaction	Writing
English	C2	C1	B2	B2	B2
Japanese	A2	A2	A2	A1	A1

CEFR levels: A1–A2 basic, B1–B2 independent, C1–C2 proficient.

Interests

Volleyball

Basketball

Hiking & camping

Crochet & DIY

Photography

Drawing & animation

Perfumes