

Adrian M. V. Brânzanic

Computational & theoretical chemist — Babeş-Bolyai University, Cluj-Napoca

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PROFILE

Computational and theoretical chemist with more than a decade of research experience bridging theory and experiment. My work combines density functional theory and methods beyond it — TD-DFT, QM/MM, molecular dynamics and non-equilibrium Green's-function transport — to explain how metals, clusters and functional molecules bind and transform. Interests span bioinorganic reactivity and metalloenzyme mechanisms, cobalamin and siroheme chemistry, boron and gold clusters, small-molecule activation, photofunctional dyes, and the foundations of quantum chemistry.

EDUCATION

- 2013 - 2020** **PhD in Chemistry (EQF 8)**
Babeş-Bolyai University, Cluj-Napoca. Computational & theoretical chemistry; advisor Prof. Radu Silaghi-Dumitrescu. Thesis defended September 2020.
- 2011 - 2013** **MSc in Chemical Engineering (EQF 7)**
Babeş-Bolyai University, Cluj-Napoca, Romania.
- 2007 - 2011** **BSc in Chemical Engineering (EQF 6)**
Babeş-Bolyai University, Cluj-Napoca, Romania.

APPOINTMENT

- present** **Researcher — “Raluca Ripan” Institute for Research in Chemistry**
Babeş-Bolyai University, Cluj-Napoca. Also with the Interdisciplinary Research Institute on Bio-Nano Sciences. Principal investigator on national research grants.

SKILLS AND SOFTWARE

Methods: DFT, TD-DFT, NEGF-DFT electron transport, multireference and semi-empirical methods, QM/MM, molecular dynamics, Monte-Carlo docking & adsorption, coarse-grained dynamics, solid-state chemistry, wavefunction analysis.

Quantum chemistry: Turbomole, ORCA, Gaussian, OpenMolcas, Dalton, Columbus, DMol³.

Molecular mechanics: Amber, GROMACS, HADDOCK, S4MPLE.

Solid state / materials: Materials Studio, Quantum ESPRESSO, CASTEP, DFTB+, ONETEP.

Analysis & visualisation: Multiwfn, TheoDORE, PyMOL, VMD, GaussView, TmoleX, Chemcraft, Chimera, Mercury, Spartan, HyperChem.

Computing: Experienced user of Linux, macOS and Windows.

RESEARCH VISITS AND SCHOOLS

- 2025**
29 Aug - 10 Sep **Lund University, Sweden**
Research stay — Ulf Ryde group.
- 2024**
4-15 Sep **Lund University, Sweden**
Research stay — Ulf Ryde group.
- 2023**
18-27 Oct **Lund University, Sweden**
Research stay — Ulf Ryde group.
- 2023**
18-24 Sep **J. Heyrovský Institute of Physical Chemistry, Prague, Czechia**
Research stay — Martin Srncic group.

- 2021**
21 Jan
Introduction to HPC and Kebnekaise — HPC2N, Umeå University, Sweden
Training course (online).
- 2020**
28 Nov – 16 Dec
Lund University, Sweden
Research stay — Ulf Ryde group.
- 2020**
7 Oct – 7 Nov
Lund University, Sweden
Research stay — Ulf Ryde group.
- 2019**
4 Apr – 1 May
University of Georgia, Athens, USA
Research stay — R. Bruce King group.
- 2019**
19–21 Jun
PT-symmetric quantum theory — lecture course by Carl M. Bender (Washington University)
Laboratoire de Chimie Théorique, Sorbonne Université, Paris, France.
- 2017**
17–20 Dec
33rd Winter School in Theoretical Chemistry, Helsinki
University of Helsinki, Finland.
- 2016**
24–28 Jul
Summer School on Molecular Boron Chemistry, Würzburg
Julius-Maximilians-University, Germany.
- 2016**
1 Jun – 4 Jul
Lund University, Sweden
Research stay — Ulf Ryde group.
- 2015**
29 Nov – 15 Dec
Lund University, Sweden
Research stay — Ulf Ryde group.
- 2015**
31 Aug – 29 Sep
Lund University, Sweden
POSDRU placement — Ulf Ryde group.
- 2015**
30 Apr – 30 May
Lund University, Sweden
POSDRU placement — Ulf Ryde group.
- 2014**
4–9 Sep
MatCatNet workshop “From Molecules to Functionalised Materials”
Ohrid, North Macedonia.
- 2014**
30 Jun – 30 Aug
SOE-DAAD placement, Leipzig University
Leipzig, Germany — Evamarie Hey-Hawkins group.

ORGANISING CONFERENCES AND SCHOOLS

- 2026**
18–20 Jun
Molecular Modeling in Chemistry and Biochemistry (MolMod), 11th edition
Organising committee, Cluj-Napoca.
- 2022 – 2023**
Molecular Modeling in Chemistry and Biochemistry (MolMod), 10th edition — online lecture series
Organising committee, Cluj-Napoca.
- 2018**
28–30 Oct
Molecular Modeling in Chemistry and Biochemistry (MolMod), 9th edition
Organising committee, Cluj-Napoca.
- 2016**
13–15 Nov
Molecular Modeling in Chemistry and Biochemistry (MolMod), 8th edition
Organising committee, Cluj-Napoca.
- 2014**
13–15 Nov
Molecular Modeling in Chemistry and Biochemistry (MolMod), 7th edition
Organising committee, Cluj-Napoca.
- 2026**
28 Sep – 2 Oct
QCES — Quantum Chemistry of Excited States International School (3rd edition)
Co-organiser, Cluj-Napoca.
- 2025**
29 Sep – 3 Oct
QCES — Quantum Chemistry of Excited States International School (2nd edition)
Co-organiser, Cluj-Napoca.
- 2024**
25–29 Nov
QCES — Quantum Chemistry of Excited States International School (1st edition)
Co-organiser, Cluj-Napoca.

2025

Symposium on Theoretical Methods Applied in Biochemistry

Organiser, Babeş-Bolyai University, Cluj-Napoca.

AWARDS

2017

Ivanovo

First prize — XI All-Russian School-Conference of Young Scientists

Oral presentation.

2017

Ivanovo

First prize — 8th Russian School-Conference of Young Scientists

Oral presentation.

LANGUAGES

Romanian — native speaker · English — C2 (proficient).

TALKS AND SEMINARS

6. Quantum Chemistry of Excited States (QCES) International School, 28 September – 2 October 2026, Cluj-Napoca, Romania. – Lecturer.
5. 25th-anniversary meeting of the Interdisciplinary Research Institute on Bio-Nano Sciences (ICI-BNS), 15 May 2026, Cluj-Napoca, Romania. – Invited talk.
4. Department of Medicinal Chemistry, University of Uppsala, Sweden, 15–22 April 2026. – Invited lecture series (two lectures).
3. Max Planck Institute for Solid State Research, Stuttgart, Germany, 15 January 2026. – Invited seminar.
2. MolMod Lectures 2022–2023 (online), Cluj-Napoca — “Exchange interactions in biochemistry” (Parts 1 & 2), 20 January and 10 February 2023. – Invited lectures.
1. Center for Computational Quantum Chemistry (CCQC), University of Georgia, Athens, USA, 2 May 2019. – Invited seminar.

CONFERENCES

21. Molecular Modeling in Chemistry and Biochemistry (MolMod 2026), 18–20 June 2026, Cluj-Napoca, Romania. – Keynote lecture.
20. International Society of Quantum Biology and Pharmacology (ISQBP) President’s Meeting, 15–18 June 2026, Cluj-Napoca, Romania. – Poster presentation.
19. Young Researchers’ International Conference on Chemistry and Chemical Engineering (YRICCCE V), 8–10 May 2025, Cluj-Napoca, Romania. – Oral presentation.
18. 14th European Conference on Computational and Theoretical Chemistry, 27–31 August 2023, Thessaloniki, Greece. – Poster presentation.
17. 20th International Conference on Biological Inorganic Chemistry, 16–21 July 2023, Adelaide, Australia. – Oral presentation.
16. 17th International Congress of Quantum Chemistry, 26 June – 1 July 2023, Bratislava, Slovakia. – Poster presentation.
15. 16th European Biological Inorganic Chemistry Conference, 17–21 July 2022, Grenoble, France. – Poster presentation.
14. Young Researchers’ International Conference on Chemistry and Chemical Engineering (YRICCCE III), 4–5 June 2021, Cluj-Napoca, Romania. – Oral presentation.
13. 9th Molecular Modeling in Chemistry and Biochemistry, 28–30 October 2018, Cluj-Napoca, Romania. – Oral presentation.
12. 35th Romanian National Chemistry Conference, 2–5 October 2018, Căciulata, Romania. – Oral presentation.
11. XI All-Russian School-Conference of Young Scientists — theoretical and experimental chemistry of liquid-phase systems, 30 October – 4 November 2017, Ivanovo, Russia. – Oral presentation, awarded 1st prize.
10. 11th Triennial Congress of the World Association of Theoretical and Computational Chemistry, 27 August – 1 September 2017, Munich, Germany. – Poster presentation.

9. 16th International Meeting on Boron Chemistry (IMEBORON XVI), 9–13 July 2017, Hong Kong, China. – Poster presentation.
8. International Conference Bio-Nano-Math-Chem, 28–30 June 2017, Cluj-Napoca, Romania. – Poster presentation.
7. 8th Russian School-Conference of Young Scientists: quantum-chemical calculations, structure and reactivity of organic and inorganic molecules, 24–26 April 2017, Ivanovo, Russia. – Oral presentation, awarded 1st prize.
6. 8th Molecular Modeling in Chemistry and Biochemistry, 13–15 November 2016, Cluj-Napoca, Romania. – Oral presentation.
5. 8th Molecular Quantum Mechanics, 26 June – 1 July 2016, Uppsala, Sweden. – Poster presentation.
4. 1st Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE I), 12–14 May 2016, Cluj-Napoca, Romania. – Oral presentation.
3. 10th European Conference on Computational Chemistry, 31 August – 3 September 2015, Fulda, Germany. – Poster presentation.
2. 7th Molecular Modeling in Chemistry and Biochemistry, 13–15 November 2014, Cluj-Napoca, Romania. – Oral presentation.
1. 33rd Romanian National Chemistry Conference, 1–3 October 2014, Căciulata, Romania. – Oral presentation.

BOOK

A. Lupan, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu. *Elemente de chimie computațională* (Elements of Computational Chemistry). Presa Universitară Clujeană, Cluj-Napoca, 2024. ISBN 978-606-37-2255-4. Open access (CC BY 4.0).

PUBLICATIONS (34 PEER-REVIEWED, 2014-2026)

An asterisk (*) marks the corresponding author.

34. M. E. Gal, C. Cristea, C. Zăgrean-Tuza, A. Turza, **A. M. V. Brânzanic**, M. Venter, L. Gaina*. New materials containing phenothiazine carboxylate salts for dual optical sensing of explosive nitroaromatics. *Dyes and Pigments* 113717 (2026).
33. S.-R. Cosma, D. Gorgan, **A. M. V. Brânzanic***, R. Silaghi-Dumitrescu*. No heme-chlorite adduct in the catalytic cycle of chlorite dismutase: QM/MM and dynamics. *J. Inorg. Biochem.* 113312 (2026).
32. R.-I. Onija, S.-R. Cosma, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Rationales for the choice of metals for super-reduced biological metal centers: cobalt in cobalamin versus nickel in F430. *Chem. Eur. J.* e71214 (2026).
31. L. J. Williams, J. J. A. G. Kamps, **A. M. V. Brânzanic**, M. Lehene, *et al.* Can ferric-oxyl excited states explain elongated iron-oxygen bonds in heme peroxidase catalytic intermediates? *Nature Communications* 17(1) (2026).
30. J. Hidalgo, L. Hidalgo, C. D. Serrano Aguiar, *et al.*, **A. M. V. Brânzanic**, N. Ignat, G. L. Turdean*. Study of Caesalpinia spinosa extracts as a green corrosion inhibitor for mild steel. *Langmuir* 41(14), 9406–9421 (2025).
29. T. R. Ovari, **A. M. V. Brânzanic**, G. Katona, G. S. Szabó*, L. M. Mureșan. New eco-friendly corrosion inhibitor for zinc based on expired Detralext drug. *Mater. Today Commun.* 46, 112739 (2025).
28. V. Lozovan, G. Borodi, I. Perhaița, A. Turza*, **A. M. V. Brânzanic**, A. Pîrnău, L. E. Mureșan. Eu(III) complexes derived from a 2-quinolinecarbohydrazide Schiff-base ligand. *J. Mol. Struct.* 1322, 140397 (2025).
27. B. Stoean (Vasile), R. Pop, D. Rugină, **A. M. V. Brânzanic**, *et al.* Photosensitizer activity of phenothiazinium derivatives against melanoma cells and DFT insights into singlet-oxygen generation. *Bioorg. Chem.* 163, 108720 (2025).
26. C. Zăgrean-Tuza, L. Pădurean, M. Lehene, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Globin ferryl species: nature of the protonation event at pH < 5? *JBIC* 30(1), 61–70 (2025).
25. M. Lehene, C. Zăgrean-Tuza, S. D. Iancu, S.-R. Cosma, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. The chlorite adduct of aquacobalamin: contrast with chlorite dismutase. *JBIC* 30(1), 25–34 (2025).
24. L. E. Mureșan*, I. Perhaița, **A. M. V. Brânzanic**, C. Saroși, L. Barbu-Tudoran, G. Borodi, I. Petean. Effect of precipitation conditions on the properties of some zinc-oxidic-based compounds. *J. Sol-Gel Sci. Technol.* 109(3), 795–809 (2024).
23. R. Doukeh, D. Crăciun, M. Lehene, **A. M. V. Brânzanic**, A. Lupan, R. Silaghi-Dumitrescu*. An iron-free nitrogenase? Ability to bind/activate N₂ in manganese and cobalt complexes. *J. Coord. Chem.* 77(12–14), 1597–1606 (2024).

22. J. Hidalgo Viteri*, N. Cotolan, A. Lupan, **A. M. V. Brânzanic**, G. L. Turdean*. A poly(methyl methacrylate)-ibuprofen composite film as anticorrosive coating of a Ti-6Al-4V surface. *J. Solid State Electrochem.* 28(2), 479-494 (2024).
21. M. Gal, L. Gaina, T. Lovász, E. Gal, A.-M. Crăciun, M. Foçsan, A. Turza, D. Rugină, **A. M. V. Brânzanic**, S. Pesek, R. Silaghi-Dumitrescu, C. Cristea*. Sonochemical synthesis and DFT of novel (N-arylamino)phenothiazinium dyes for fluorescence cell imaging. *Spectrochim. Acta A* 322, 124768 (2024).
20. **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu. Quale mechanics as a metaphysical Weltanschauung of quantum mechanics. *Hist. Sci. Technol.* 13(1), 10-33 (2023).
19. R. Doukeh, D. Crăciun, A. Lupan, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Effect of the coordination environment on the ability of iron to bind/activate N₂. *Polyhedron* 243, 116571 (2023).
18. A. Gaina-Gardiuta, A. Lupan, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Cobalamin adducts with cysteine and its oxidized sulfenic, sulfinic and sulfonic derivatives. *Rev. Roum. Chim.* 68(3-4), 143-152 (2023).
17. M. Lehene, C. Zăgrean-Tuza, N. Hădade, A. Aghion, R. Şeptelean, S. D. Iancu, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. A complex of cobalamin with an organic peroxide. *New J. Chem.* 47(39), 18178-18185 (2023).
16. M. Lehene, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. The adducts of cyano- and aquacobalamin with hypochlorite. *JBIC* 28(6), 583-589 (2023).
15. B. Stoean, L. Gaina, C. Cristea*, R. Silaghi-Dumitrescu, **A. M. V. Brânzanic**, et al. New methylene-blue analogues with N-piperidiny-carbinol units. *Dyes and Pigments* 205, 110460 (2022).
14. S. Pesek, M. Lehene, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. On the origin of the blue colour in the iodine/iodide/starch supramolecular complex. *Molecules* 27(24), 8974 (2022).
13. F. Carrascoza, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. The dynamics of hemerythrin and hemerythrin derivatives. *Studia UBB Chemia* 66(4), 397-404 (2021).
12. I. Irsai, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Polylactic-acid interactions with bioceramic surfaces. *Studia UBB Chemia* 66(3), 107-121 (2021).
11. I. A. Dereven'kov*, S. V. Makarov, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu, P. A. Molodtsov, E. A. Pokrovskaya. Formation of hydroxyl radical in aqueous solutions containing selenite and glutathione. *Polyhedron* 198, 115072 (2021).
10. M. Lehene, D. Pleşa, S. Ionescu-Zincă, S. D. Iancu, N. Leopold, S. V. Makarov, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Adduct of aquacobalamin with hydrogen peroxide. *Inorg. Chem.* 60(17), 12681-12684 (2021).
9. I. A. Dereven'kov*, L. Hannibal, P. A. Molodtsov, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu, S. V. Makarov. Kinetic, spectroscopic and in-silico characterization of the first step of the reaction between glutathione and selenite. *Inorg. Chim. Acta* 499, 119215 (2020).
8. **A. M. V. Brânzanic**, U. Ryde, R. Silaghi-Dumitrescu*. Importance of the iron-sulfur component and of the siroheme modification in the resting state of sulfite reductase. *J. Inorg. Biochem.* 203, 110928 (2020).
7. A. A. A. Attia, **A. M. V. Brânzanic**, A. Muñoz-Castro*, A. Lupan*, R. B. King*. Cationic gold clusters with eight valence electrons: possible spherical aromatic systems with sigma holes. *Phys. Chem. Chem. Phys.* 21(32), 17779-17785 (2019).
6. **A. M. V. Brânzanic**, U. Ryde, R. Silaghi-Dumitrescu*. Why does sulfite reductase employ siroheme? *Chem. Commun.* 55(93), 14047-14049 (2019).
5. M. Surducun*, **A. M. V. Brânzanic**, R. Silaghi-Dumitrescu*. Heme Fe-SO₂ intermediates in sulfite reduction: contrasts with Fe-OO species from oxygen-oxygen bond-activating systems. *Int. J. Quantum Chem.* 118(19), e25697 (2018).
4. **A. M. V. Brânzanic**, A. Lupan*, R. B. King*. Dimetallaborane analogues of the octaboranes Cp₂M₂B₆H₁₀: structural variations with the skeletal electron count. *Dalton Trans.* 45(22), 9354-9362 (2016).
3. **A. M. V. Brânzanic**, A. Lupan*, R. B. King*. Dimetallaborane analogues of pentaborane. *Dalton Trans.* 44(16), 7355-7363 (2015).
2. **A. M. V. Brânzanic**, A. Lupan*, R. B. King*. The Wade-Mingos rules in seven-vertex dimetallaborane chemistry: hydrogen-rich Cp₂M₂B₅H₉ systems. *J. Organomet. Chem.* 792, 74-80 (2015).
1. **A. M. V. Brânzanic**, A. Lupan*, R. B. King*. Six-vertex hydrogen-rich Cp₂M₂B₄H₈ dimetallaboranes of the second- and third-row transition metals. *Organometallics* 33(22), 6443-6451 (2014).

RESEARCH GRANTS AND PROJECTS

- 2023 - 2025** **Promotion of intramolecular electron-transfer routes within oxygen-carrying biomolecules to counter autoxidation**
Principal investigator.
- 2024 - 2026** **Targeted tumour therapy with multifunctional platinum(IV)-drug conjugates (T3Pt)**
PNRR-III-C9-2023-I8-CF · team member.
- 2022 - 2024** **Reactivity of peripheral heme toward sulfur- and oxygen-based stressors**
PN-III-P1-1.1-PD-2021-0279 · principal investigator.
- 2020 - 2021** **Three unresolved aspects of the sulfite-reductase active site**
GTC-32141/2020 · principal investigator.
- 2020 - 2022** **Semi-artificial oxygen carriers**
PN-III-P2-2.1-PED-2019-2293 · team member.
- 2017** **Research-mobility project**
PN-III-P1-1.1-MC-2017-2121 · project leader.
- 2017 - 2019** **Molecular metal clusters: a bridge between small molecules and nanocrystals**
PN-III-P4-ID-PCE-2016-0089 · team member.
- 2015 - 2017** **Polyhedral metallaboranes: metal clusters stabilised in borane matrices**
PN-II-RU-TE-2014-4-1197 · team member.
- 2013 - 2016** **Redox activation of small molecules by biologically relevant metal centres**
PN-II-ID-PCE-2012-4-0488 · team member.