



## Adrian M.V. Brânzanic

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**Email address:** [adrian.branzanic@ubbcluj.ro](mailto:adrian.branzanic@ubbcluj.ro)

**Phone number:** (+40) 748127834

**Gender:** Male **Date of birth:** 15/02/1988 **Nationality:** Romanian

### EDUCATION AND TRAINING

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[ 30/09/2007 – 30/06/2011 ] **B. Sc. in Chemical Engineering**

*Babeş-Bolyai University*

**Address:** Cluj-Napoca, Romania

**Level in EQF:** EQF level 6

[ 30/09/2011 – 30/06/2013 ] **M. Sc. in Chemical Engineering**

*Babeş-Bolyai University*

**Address:** Cluj-Napoca, Romania

**Level in EQF:** EQF level 7

[ 30/09/2013 – 23/09/2020 ] **PhD in Chemistry**

*Babeş-Bolyai University*

**Address:** Cluj-Napoca, Romania

**Level in EQF:** EQF level 8

[ 30/06/2014 – 30/08/2014 ] **SOE-DAAD placement**

*Leipzig University*

**Address:** Leipzig, Germany

[ 04/09/2014 – 09/09/2014 ] **MatCatNet Workshop “From Molecules to Functionalised Materials”**

**Address:** Ohrid, North Macedonia

[ 30/04/2015 – 30/05/2015 ] **POSDRU placement**

*Lund University*

**Address:** Lund, Sweden

[ 31/08/2015 – 29/09/2015 ] **POSDRU placement**

*Lund University*

**Address:** Lund, Sweden



[ 29/11/2015 – 15/12/2015 ] **Research Stay**

*Lund University*

**Address:** Lund, Sweden

[ 01/06/2016 – 04/07/2016 ] **Research Stay**

*Lund University*

**Address:** Lund, Sweden

[ 24/07/2016 – 28/07/2016 ] **Summer School on Molecular Boron Chemistry**

*Julius-Maximilians-University*

**Address:** Wurzburg, Germany

[ 17/12/2017 – 20/12/2017 ] **33rd Winter School in Theoretical Chemistry - Molecular Energy and Electron Transfer**

*University of Helsinki*

**Address:** Helsinki, Finland

[ 04/04/2019 – 01/05/2019 ] **Research Stay**

*University of Georgia*

**Address:** Athens, United States

[ 07/10/2020 – 07/11/2020 ] **Research Stay**

*Lund University*

**Address:** Lund, Sweden

[ 28/11/2020 – 16/12/2020 ] **Research Stay**

*Lund University*

**Address:** Lund, Sweden

## LANGUAGE SKILLS

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**Mother tongue(s):** Romanian

**Other language(s):**

**English**

**LISTENING C2 READING C2 WRITING C2**

**SPOKEN PRODUCTION C2 SPOKEN INTERACTION C2**



## PUBLICATIONS

[ 2014 ]

Brânzanic, A. M. V.; Lupan, A.; King, R. B. Six-Vertex Hydrogen-Rich Cp<sub>2</sub>M<sub>2</sub>B<sub>4</sub>H<sub>8</sub> Dimetallaboranes of the Second- and Third-Row Transition Metals: Effects of Skeletal Electron Count on Preferred Polyhedra. *Organometallics* 2014, 33, 6433–6451.

<https://doi.org/10.1021/om500801e>

[ 2015 ]

Brânzanic, A. M. V.; Lupan, A.; King, R. B. The Wade-Mingos Rules in Seven-Vertex Dimetallaborane Chemistry: Hydrogen-Rich Cp<sub>2</sub>M<sub>2</sub>B<sub>5</sub>H<sub>9</sub> Systems of the Second and Third Row Transition Metals. *J. Organomet. Chem.* 2015, 792, 74–80.

<https://doi.org/10.1016/j.jorganchem.2015.02.030>

[ 2015 ]

Brânzanic, A. M. V.; Lupan, A.; King, R. B. Dimetallaborane Analogues of Pentaborane. *Dalt. Trans.* 2015, 44 (16), 7355–7363.

<https://doi.org/10.1039/C5DT00143A>

[ 2016 ]

Brânzanic, A. M. V.; Lupan, A.; King, R. B. Dimetallaborane Analogues of the Octaboranes of the Type Cp<sub>2</sub>M<sub>2</sub>B<sub>6</sub>H<sub>10</sub>: Structural Variations with Changes in the Skeletal Electron Count. *Dalt. Trans.* 2016, 45 (22), 9354–9362.

<https://doi.org/10.1039/C6DT00985A>

[ 2018 ]

Surducă, M.; Brânzanic, A. M. V.; Silaghi-Dumitrescu, R. Heme Fe-SO<sub>2</sub>-Intermediates in Sulfite Reduction: Contrasts with Fe-OO<sub>2</sub>-Species from Oxygen-Oxygen Bond Activating Systems. *Int. J. Quantum Chem.* 2018, 118 (19), 2–10.

<https://doi.org/10.1002/qua.25697>

[ 2019 ]

Attia, A. A. A.; Brânzanic, A. M. V.; Muñoz-Castro, A.; Lupan, A.; King, R. B. Cationic Gold Clusters with Eight Valence Electrons: Possible Spherical Aromatic Systems with Sigma Holes. *Phys. Chem. Chem. Phys.* 2019, 21 (32), 17779–17785.

<https://doi.org/10.1039/c9cp03440d>

[ 2019 ]

Dereven'kov, I. A.; Hannibal, L.; Molodtsov, P. A.; Brânzanic, A. M. V.; Silaghi-Dumitrescu, R.; Makarov, S. V. Kinetic, Spectroscopic and in Silico Characterization of the First Step of the Reaction between Glutathione and Selenite. *Inorganica Chim. Acta* 2019, 499 (October 2019), 119215. <https://doi.org/10.1016/j.ica.2019.119215>.

<https://doi.org/10.1016/j.ica.2019.119215>



[ 2019 ]

**Brânzanic, A. M. V.; Ryde, U.; Silaghi-Dumitrescu, R. Importance of the Iron – Sulfur Component and of the Siroheme Modification in the Resting State of Sulfite Reductase. J. Inorg. Biochem. 2019, 203, 110928.**

<https://doi.org/10.1016/j.jinorgbio.2019.110928>

[ 2019 ]

**Brânzanic, A. M. V.; Ryde, U.; Silaghi-Dumitrescu, R. Why Does Sulfite Reductase Employ Siroheme? Chem. Commun. 2019, 55, 14047–14049.**

<https://doi.org/10.1039/c9cc05271b>

[ 2021 ]

**Carrascoza, F.; Brânzanic, A. M. V.; Silaghi-Dumitrescu, R. The Dynamics of Hemerythrin and Hemerythrin Derivatives. Stud. Univ. Babeş-Bolyai Chem. 2021, 66 (4), 397–404.**

<https://doi.org/10.24193/subbchem.2021.4.29>

[ 2021 ]

**Dereven'kov, I. A.; Makarov, S. V.; Brânzanic, A. M. V.; Silaghi-Dumitrescu, R.; Molodtsov, P. A.; Pokrovskaya, E. A. Formation of Hydroxyl Radical in Aqueous Solutions Containing Selenite and Glutathione. Polyhedron 2021, 198, 115072.**

<https://doi.org/10.1016/j.poly.2021.115072>

[ 2021 ]

**Irsai, I.; Brânzanic, A. M. V.; Silaghi-dumitrescu, R. Polylactic Acid Interactions with Bioceramic Surfaces. Stud. Univ. Babeş-Bolyai Chem. 2021, LXVI (3), 107–121.**

<https://doi.org/10.24193/subbchem.2021.3.06>

[ 2021 ]

**Lehene, M.; Plesa, D.; Ionescu-Zinca, S.; Iancu, S. D.; Leopold, N.; Makarov, S. V.; Brânzanic, A. M. V.; Silaghi-Dumitrescu, R. Adduct of Aquacobalamin with Hydrogen Peroxide. Inorg. Chem. 2021, 1–4.**

<https://doi.org/10.1021/acs.inorgchem.1c01483>

## CONFERENCES AND SEMINARS

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### Conferences

**14.** Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE III), 4-5 June, 2021 Cluj-Napoca, Romania. - Oral presentation.

**13.** 9<sup>th</sup> Molecular Modeling in Chemistry and Biochemistry, 28-30 October 2018, Cluj-Napoca, Romania. - Oral presentation.

**12.** A XXXV-a Conferinta Nationala de Chimie, Caciulata, Romania, 2-5 October **2018**. - Oral presentation.

**11.** The XI All-Russian School-Conference of Young Scientist - Theoretical and experimental chemistry of liquid-phase systems, Ivanovo, Russia, 30 October - 4 November 2017- Oral presentation, **awarded 1<sup>st</sup> prize**.



10. 11<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemistry, Munich, Germany, 27 August – 1 September **2017**. – Poster presentation.
9. 16<sup>th</sup> International Meeting on Boron Chemistry (IMEBORON XVI), Hong Kong, China, 9-13 July **2017**. – Poster presentation.
8. International Conference Bio-Nano-Math-Chem, Cluj-Napoca, Romania, 28-30 June **2017**. – Poster presentation.
7. 8<sup>th</sup> Russian School-Conference of Young Scientists: "Quantum-chemical calculations. Structure and reactivity of organic and inorganic molecules", Ivanovo, Russia, 24-26 April **2017**. - Oral presentation, **awarded 1<sup>st</sup> prize**.
6. 8<sup>th</sup> Molecular Modeling in Chemistry and Biochemistry, Cluj-Napoca, 13-15 November, **2016**. – Oral presentation.
5. 8<sup>th</sup> Molecular Quantum Mechanics, Uppsala, Sweden, 26 June – 1 July **2016**. – Poster presentation.
4. 1<sup>st</sup> Young Researchers' International Conference on Chemistry and Chemical Engineering, Cluj-Napoca, Romania, 12-14 May **2016**. – Oral presentation.
3. 10<sup>th</sup> European Conference on Computational Chemistry, Fulda, Germany, 31 August – 3 September **2015**. – Poster presentation.
2. 7<sup>th</sup> Molecular Modeling in Chemistry and Biochemistry, Cluj-Napoca, 13-15 November, **2014**. – Oral presentation.
1. A XXXIII-a Conferinta Nationala de Chimie, Caciulata, Romania, 1-3 October **2014**. - Oral presentation.

## JOB-RELATED SKILLS

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### Job-related skills

- Electronic structure calculations
- Predominantly DFT
- Semiempirical
- Basic multireference methods
- Molecular Mechanics
- Molecular dynamics (simple, quench and annealing dynamics)
- Monte Carlo related methods ( adsorbtion, docking )
- Coarse Grain dynamics ( experience only with the Martini force field )
- QM/MM (medium experience)
- Related software packages:
- Experienced with Gaussian, Turbomole, Materials Studio (Forcite, Mesocite, MesoDyn, GULP, VAMP, Sorption, Conformers, Adsorbtion Locator, Amorphous Cell, CASTEP,DFTB+,DMol3), Spartan, Orca, Amber, Hyperchem, Chemcraft, Chimera, ViewerLite, Molden, Mercury, Multiwfn.
- Basic with Jimp2, Mopac, Molcas, WebMO.
- Programming skills
- Experienced use of UNIX and Linux based enviroments.

## PROJECTS

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[ 01/09/2013 – 01/09/2016 ]

### Activarea redox a moleculelor mici de catre centri metalici cu relevanta biologica - PN-II-ID-PCE-2012-4-0488

Team member



[ 01/10/2015 – 02/10/2017 ]

**Metalaborani poliedrali: clusteri metalici stabilizați în matrici boranice - PN-II-RU-TE-2014-4-1197**

Team member

[ 01/07/2017 – 01/07/2019 ]

**Clusteri metalici moleculari: o punte între molecule mici și nanocristale - PN-III-P4-ID-PCE-2016-0089**

Team member

[ 18/12/2017 – 21/12/2017 ] **Proiect de mobilitate - PN-III-P1-1.1-MC-2017-2121**

Project leader

[ 01/11/2020 – 31/10/2022 ] **Transportori semi-artificiali de oxigen - PN-III-P2-2.1-PED-2019-2293**

Team member

[ 15/06/2020 – 14/06/2021 ]

**Explorarea teoretică a trei aspecte rămase neelucidate în situl activ al Sulfit Reductazei: cuplajul magnetic interfactorial, mecanismul de reducere a sulfitului la sulfură și mecanismul de reducere a nitritului la amoniac - GTC-32141/2020**

Project leader

[ 01/04/2022 – 31/03/2024 ]

**Reactivitatea hemului periferic către agenți de stres bazați pe sulf și oxigen - PN-III-P1-P1-1.1-PD-2021-0279**

Project leader