Dr. Alexandra Bargan

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Brainmap codes: (UEFISCDI ID (UEF-iD): **U-1700-039Q-1815**

Research topics

Specialist in the field of chemistry, subdomains polymer chemistry/inorganic chemistry, with experience in materials characterization using methods such as: infrared spectroscopy, proton and carbon nuclear magnetic resonance, single crystal X-ray diffraction, thermogravimetric measurements, X-ray fluorescence, dynamic vapour sorption and surface tension measurements, scanning electron microscopy, atomic force microscopy, differential scanning calorimetry etc. The research activity is focused on synthesis and characterization of new silicon compounds; functionalized silica nanostructures; new zwitterionic siloxane compounds with interesting properties, new Schiff Base-type ligands derived from silicon compounds and their metal complexes, synthesis of functionalized silica nanostructures and preparation of silicone composites, new metal-organic frameworks with catalytic activity, new biopolymer nanocomposites with antibacterial activity, new cellulose-siloxane hybrid materials. A part of the research activity is also focused on development of modeling and optimization strategies based not only on molecular modeling but also on neural models (NN), genetic algorithms and fuzzy logic for synthesis/characterization of new silicon compounds and functionalized silica nanostructures. The artificial intelligence tools were applied for modeling and optimization of different processes from silicone chemistry and environmental protection. The NN were used to optimize the synthesis processes by inverse neural network modeling.

Scientific research

Author and co-author of **74 ISI articles** (**36** in Q1 zone and **20** in Q2 zone), **4 book chapters**, **6** articles in proceedings, **2** patent applications, **50** posters, **30** oral communications, special prize, 2 gold and 1 silver medals at international conference INVENTICA, member in **20 research national/international grants** and **Project Leader** for 1 national grant (Contract type „PED", PN-III-P2-2.1-PED-2021-3900, „Intelligent tools for design, processing and optimization of new PS-POSS-IL (polysulfone-silsesquioxanes impregnated with ionic liquids) type membranes applied in CO_2 gas separation", AI-Syn-PPOSS*:* PN-III-P2-2.1-PED-2021-3900), 672 citations (HI = 17).

Visibility

https://www.brainmap.ro/alexandra-bargan-nistor ; https://orcid.org/0000-0002-9433-9595 ; https://www.webofscience.com/wos/author/record/B-8981-2019; https://scholar.google.com/citations?hl=en&user=FW1vhAIAAAAJ&view_op=list_works&sortby=pubdate ; https://www.webofscience.com/wos/author/record/B-8981-2019

SELECTED RELEVANT SCIENTIFIC ARTICLES

1. Bargan, A., Onofrei, M.D., Stoica, I., Doroftei, F., Dunca, S., Filimon, A., „Materials based on Quaternized Polysulfones with potential applications in biomedical field: structure-properties relationship", *International Journal of Molecular Sciences*, **2022**, 23(9), 4721, https://doi.org/10.3390/ijms23094721 , F.I.=5.924, (Q2).

2. David, G., **Bargan, A.,** Drobota, M., Bele, A., Rosca, I., "Comparative Investigation of Collagen-Based Hybrid 3D Structures for Potential Biomedical Applications", *Materials*, **2021**, 14(12), 3313, https://doi.org/10.3390/ma14123313, F.I.=3.623, (Q1).

3. Bargan, A., Cazacu, M., Dascalu, M., Macsim, A.M., Soroceanu, A., Macsim, I.F., „Synthesis, structural characterization and properties evaluation of two new zwitterionic siloxane compounds", *Polyhedron*, **2020**, 179, 114356, https://doi.org/10.1016/j.poly.2020.114356 , F.I. =2.284, (Q2).

4. Bargan, A., Zaltariov, M.F., Vlad, A., Dumitriu, A.M.C., Soroceanu, A., Macsim, A.M., Dascalu, M., Varganici, C.D., Cazacu, M., Shova, S., „Keto-enol tautomerism in new silatranes Schiff bases tailed with different substituted salicylic aldehyde", *Arabian Journal of Chemistry*, **2020**, 13 (1), 3100-3111, https://doi.org/10.1016/j.arabjc.2018.09.001, F.I.=3.298, (Q2).

5. Ciubotaru, B.I., Zaltariov, M.F., Dascalu, M., Bele, A., **Bargan, A**., Cazacu, M., „ Amino-functionalized silicones processed as porous dual covalent/supramolecular networks for pressure sensing" *Reactive and Functional Polymers* **2024**, 194, 105792 (FI = 5.1), (Q1)

6. Zaltariov, M.F., Turtoi, M., Peptanariu, D., Macsim, A.M., Clima, L., Cojocaru, C., Vornicu, N., Ciubotaru, B.I., **Bargan, A.,** Calin, M., Cazacu, M., „Chemical attachment of 5-nitrosalicylaldimine motif to silatrane resulting in an organic-inorganic structure with medicinal significance", *Pharmaceutics* **2022**, 14(12), 2838, https://doi.org/10.3390/pharmaceutics14122838 , (FI= 6.525) (Q1).

7. Cazacu, M., Racles, C., Zaltariov, M. F., Dascalu, M., Bele, A., Tugui, C., **Bargan, A.,** Stiubianu, G., From amorphous silicones to Si-containing highly ordered polymers: some Romanian contributions in the field, *Polymers* **2021**, 13(10), 1605, https://doi.org/10.3390/polym13101605 , F.I.=4.329, (Q1).

Specializations and qualifications:

- „Physics of Advanced Materials Winter School", Thessaloniki, Greece, January **2008**
- "The CAMD Summer School - Electronic Structure Theory and Materials Design" Lyngby - Copenhaga, Danemarca, August **2008**
- Research Stage on using the X-ray Spectrometer X-Calibur SDD, for analyzing the solids, liquids and powder materials, **2011**.
- Two research stages on Single Crystal X-ray Diffraction at ICT, Germany, March **2012**, February **2013** within the project STREAM- contract nr. 264115- European Union's Seventh Framework Programme (FP7/2007–2013)
- „How to write a successful Horizont 2020 project", Iasi, 10-13 october **2016**.
- Two research stages on synthesis and advanced characterization of new ligands and Fe(II) and Fe(III) complexes with spin crossover properties, at SRL Polivalent-95, in Chisinau, Moldova, November **2019**, September **2020** within the project "Multifunctional Spin Crossover Materials" H2020-MSCA-RISE-2016, SPINSWITCH, No 734322/ (dr. Sergiu Shova).

Awards:

- Dynamic dual mode materials for human thermal comfort; G. Stiubianu, **A. Bargan**, M. Dascalu, B. Adrian, T. Codrin, C. Ursu, C. Racles, M. Cazacu; INVENTICA 2022, Inventics International Conference, The 26th edition 22-24.06.2022, Iasi, Romania (poster –silver medal)
- Intelligent tools for design, processing and optimization of new PS-POSS-IL (polysulfone-silsesquioxanes impregnated with ionic liquids) type membranes applied in CO_2 gas separation; **A. Bargan**, M. Dascalu, G. Stiubianu, B. Adrian, C. Cojocaru, A. Filimon, A. Dobos, A. Soroceanu, A. M. Macsim, M. Cazacu, INVENTICA 2023, Inventics International Conference, The 27th edition 21-23.06.2023, Iasi, Romania (poster –gold medal)
- Process for obtaining the polysulfone membranes functionalized with ionic liquids applicable in technological processes of water treatment by microfiltration; A. Filimon, A. Dobos, **A. Bargan**, L.Lupa, patent aplication OSIM: A/00466/1.08.2022, INVENTICA 2023, Inventics International Conference, The 27th edition 21-23.06.2023, Iasi, Romania (gold medal/premiu special),