

## Curriculum Vitae

**Dr. hab. Cina Foroutan-Nejad, Ph.D.**



*Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224, Warsaw, Poland*

## 1. Education and Training

### Education

- 2005–2011** Ph.D. in Computational Organic Chemistry under Supervision of Prof. Parviz Rashidi-Ranjbar and Dr. Shant Shahbazian  
University of Tehran  
Thesis Title: Magnetic aromaticity: from NICS to bond magnetizability  
Specialization Theoretical and Computational Chemistry
- 2002–2005** M.Sc. in Physical Organic Chemistry under Supervision of Prof. Parviz Rashidi-Ranjbar and Dr. Ebrahim Kianmehr  
University of Tehran  
Thesis Title: Ring expansion reaction of 9,9-dichloro-9,9 a- dihydro- cyclopropano [c] pyrene: a mechanistic study  
Specialization Reaction Mechanisms and Computational Chemistry
- 1998–2002** B.Sc. in Applied Chemistry  
Azad University, Tehran, Central Branch

## 2. Employment

### December 2020 – Current:

Associate Professor at  
Institute of Organic Chemistry, Polish Academy of Sciences

### January 2021 – 2024:

Research advisor at  
Institute of Organic Chemistry and Biochemistry, Czech Academy of Science

### January 2020 – December 2020:

Principle Investigator at  
Department of Chemistry, Faculty of Science, Masaryk University & National Centre for Biomolecular Research, Faculty of Science, Masaryk University, 625 00 Brno, Czech Republic

### December 2014 – December 2019:

Principle Investigator at  
CEITEC – Central European Institute of Technology, Masaryk University, Kamenice 5/A4, CZ-625 00, Brno, Czech Republic

### October 2012 – November 2014:

Postdoctoral researcher at  
National Centre for Biomolecular Research, Faculty of Science, Masaryk University, 625 00 Brno, Czech Republic

### September 2008 – October 2012

Lecturer at  
School of Chemistry, College of Science, University of Tehran, Tehran, Iran

## 3. Honors and Awards

- 2000 Young Scientist Award at the Azad University for Designing new energetic materials  
2001 Ranked 8 among about 9000 participants at the national chemistry Olympiad  
2006 Ranked 1 in the PhD entrance exam of the University of Tehran and of Tarbiat Modares University  
2018 GAMU-E grant for excellent scientific results at the Masaryk University  
2021 Director's award of the Polish Academy of Sciences for scientific achievements  
2022 Director's award of the Polish Academy of Sciences for scientific achievements  
2023 Director's award of the Polish Academy of Sciences for scientific achievements  
2024 MEiN Award for research by the Minister of Science and Technology of Poland

2024 Director's award of the Polish Academy of Sciences for scientific achievements

#### 4. Teaching Experience

- 8- 2020-Current Introduction to Computational Chemistry at Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland.
- 7- 2012-2020 Chemical Bond Theory at Department of Chemistry, Masaryk University, Brno, Czechia.
- 6- 2012-2020 Introduction to Computational Chemistry at Department of Chemistry, Masaryk University, Brno, Czechia.
- 5- 2011-2012 General Chemistry at Department of Chemistry, the University of Tehran, Iran.
- 4- 2009-2011 General Chemistry and Organic Chemistry at Department of Biology, the University of Tehran, Iran.
- 3- 2008-2011 General Chemistry at Department of Physics, the University of Tehran, Tehran, Iran.
- 2- 2004-2008 General Chemistry at Department of Physics, Shahed University, Tehran, Iran.
- 1- 2002-2004 Chemistry at Mofid High school, Tehran, Iran.

#### 5. Research Funding

<b>2021-2025</b>	2,200,600 PLN OPUS (60 months)
<b>2020-2023</b>	<u>Co-Applicant</u> 5,400,000 CZK, Ministry of Education, Czech Republic (GACR) (36 Months)
<b>2018-2019</b>	420,000 CZK, GAMU E, Prize for excellent results
<b>2017-2020</b>	3,615,000 CZK, Ministry of Education, Czech Republic (GACR) (36 Months)
<b>September 2014</b>	2,000 € Award from Center of Theoretical and Computational Chemistry (CTCC), Norway, for covering research stay in Norway
<b>2014-2017</b>	129,558 € Marie Curie Fellowship (26 Months)

#### 6. Internships, and Scientific Stays

##### November 2013 and September 2014

Visiting Researcher at group of Kenneth Ruud, UiT The Arctic University of Norway, Tromso, Norway  
May - July 2014:

Visiting Researcher at group of Petr Bouř, Institute of Organic Chemistry and Biochemistry of the Academy of Sciences of the Czech Republic

October 2012 – November 2014:

Postdoctoral researcher at group of Radek Marek, National Centre for Biomolecular Research, Faculty of Science, Masaryk University, 625 00 Brno, Czech Republic

#### 7. Mentoring Activity

My team at IOCPAS currently is composed of 2 postdoctoral researchers (Mahdi Sasar a solid state physicist working on memristive devices) and Emran Masoumifeshani (a computational chemist that focuses on basic research), and two PhD students (Minu Sheeja and Muhammad Yasir Mehboob).

-**Supervisor** of Ph.D. Thesis Minu Sheeja

Topic: Synthesis of artificial amino acids for brain inspired electronics (No Publication So Far)

-**Supervisor** of Ph.D. Thesis Muhammad Yasir Mehboob

Topic: Design of molecular electronic devices (Publications No. 77)

-**Supervisor** of Ph.D. Thesis Martin Novák

Topic: Effect of external electric fields on chemical bonding (Publications No. 24, 25, 31, 32, 35, and 36)

-**Supervisor** of Ph.D. Thesis Esmacil F. Bonab

Topic: Designing molecular devices based on endohedral fullerenes (Publications No. 38 and 49)

-**Supervisor** of Ph.D. Thesis Vojtech Šadek

Topic: Chemical bonding from the perspective of the theory of Interacting Quantum Atoms (Publication No. 59)

-**Co-Supervisor** of Ph.D. Thesis Ben J. R. Cuyacot

Topic: Interpretation of magnetic response properties of heavy metal complexes (Publications No. 54, 58 and 64)

-**Advisor** of Ph.D. Thesis Pankaj L. Bora

Topic: The effect of intermolecular interactions on magnetic properties of molecules (Publication No. 38)

-**Supervisor** of M.Sc. Thesis Jan Michal Kormanik

Topic: Assessing the relationship between aromaticity and conductivity among porphyrinoids

-**Supervisor** of B.Sc. Thesis Tomaš Janda

Topic: Surveying energetic and magnetic properties of C<sub>6</sub>H<sub>6</sub> isomers (Publication No. 39)

## 8. Reviewing Activity

**Review Editor** of **Frontiers of Chemistry**, Nature Publishing Group

**Reviewer** of 440+ manuscripts at Science, Journal of the American Chemical Society, Angewandte Chemie, Nature Communications, Inorganic Chemistry, ACS Applied Nano Materials, and many more.

Full list of reviewing activity is available at WoS:

<https://www.webofscience.com/wos/author/record/I-7512-2013>

**Distinguished Reviewer in Years 2016, 2017, and 2018 According to Publons Statistics**

## 9. Summary of Scientometrics Information

Number of ISI Journal Publications:

78 (7 in 2023, 5 in 2024, and 2 in 2025)

Corresponding author in 52 publications

Number of Single-Author Publications: 7 (2 in JPC A, 1 in PCCP, 1 in Theor. Chem. Acc., 1 in Angew. Chem. Int. Ed., 1 in Nature Communications, and 1 in JOC)

Number of Invited Papers: 5 (3 in JPC A, 1 in PCCP, 1 in OBC, 1 in Nature)

Number of publications in M.Sc.: 2 (Publications No. 1 and 2)

Number of publications in Ph.D.: 8 (Publications No. 3 to 10)

Full list of publications available at:

<https://scholar.google.com/citations?user=tc6ZQV4AAAAJ&hl=en>

Invited Talks: 18

H-Index: 29 (WoS) / 29 (Scopus) / 32 (Google Scholar)

Number of Citations: 2300+ (WoS), 2300+ (Scopus) 2800+ (Google Scholar)

## 10. List of Publications in Impacted Journals According to Web of Science

- **The asterisks (\*) denotes the corresponding author(s).**

**78-** One-Pot Transition-Metal-Free Synthesis of  $\pi$ -Extended Bipolar Polyaromatic Hydrocarbons, K.

Bartkowski, E. Masoumifeshani, U. Klimczak, M. Kotowska, B. Furman, **C. Foroutan-Nejad\***, M. Lindner\*, **Angew. Chem. Int. Ed.** 2025, 64, e202423282.

**77-** Indoloindolizines: The Complete Story of a Polycyclic Aromatic Scaffold from Theoretical Design to Organic Field-Effect Transistor Applications, A. Pareek, M. Y. Mehboob, M. Cieplak, M. Majdecki, H. Szabat, K. Noworyta, P. Polczyński, M. Morawiak, P. S. Sharma, **C. Foroutan-Nejad\***, Przemysław Gawel\*, **J. Am. Chem. Soc.**, 2025, 147, 5996-6005.

**76-** Reply to: An approach to the resolution of the dispute on collective atomic interactions, N. A. G.

Bandeira\*, Á. Martín-Pendás\*, **C. Foroutan-Nejad\***, **Nat. Commun.**, 2024, 15, 10403.

- 75- Classical versus Collective Interactions in Asymmetric Trigonal Bipyramidal Alkaline Metal-Boron Halide Complexes, Z Badri, **C Foroutan-Nejad\***, *Chem. Eur. J.*, 2024, 30, e202400156.
- 74- Aromaticity of Actinides on the Edge of the Periodic Table. Z Badri, **C Foroutan-Nejad\***, *Nat. Rev. Chem.*, 2024, 8, 551-560.
- 73- Tetraquinolines; Four Linked Quinoline Units or Porphyrinoids. Z Badri, F Nouri, **C Foroutan-Nejad\***, *Org. Biomol. Chem.*, 2024, 22, 2284-2291.
- 72- Alkaline earth metal-assisted dinitrogen activation at nickel. T. Knoell, J. Polanco, S. N. MacMillan, J. A. Bertke, **C. Foroutan-Nejad\***, K. Lancaster\*, G. Bakhoda\*, *Dalton*, 2024, 53, 4689-4697.
- 71- Anti-electrostatic Cation··· $\pi$ -Hole and Cation···lp-Hole Interactions Are Stabilized via Collective Interactions. R. Pino-Rios\*, R. Báez-Grez, **C. Foroutan-Nejad\***, *Chem. Commun.*, 2024, 60, 400-403.
- 70- Carbon rings push limits of chemical theories. P Gawel\*, **C Foroutan-Nejad\***, *Nature*, 2023, 623, 922-924
- 69- Magnetic Antiaromaticity—Paratropicity—Does Not Necessarily Imply Instability. **C. Foroutan-Nejad\***, *J. Org. Chem.* 2023, 88, 14831-14835.
- 68- Spinristor: A Spin-Filtering Memristor, A. Jaroš, M. Sasar, L. Tučková, E. F. Bonab, Z. Badri, M. Straka\*, **C. Foroutan-Nejad\***, *Adv. Electron. Mater.*, 2023, 9, 2300360.
- 67- Reply to: On the existence of collective interactions reinforcing the metal-ligand bond in organometallic compounds. V. Šádek, S. Sowlati-Hashjin, A. Sadjadi, M. Karttunen, A. Martin-Pendas\*, **C. Foroutan-Nejad\***, *Nat. Commun.*, 2023, 14, 3873.
- 66- A quest for ideal electric field-driven MX@C70 endohedral fullerene memristors: which MX fits the best? L. Tučková, A. Jaroš, **C. Foroutan-Nejad\***, M. Straka\*, *Phys. Chem. Chem. Phys.*, 2023, 25, 14254-14256.
- 65- Aromaticity: Quo Vadis. G. Merino\*, M. Solà\*, I. Fernandez\*, **C. Foroutan-Nejad\***, P. Lazzeretti\*, G. Frenking\*, H. L. Anderson, D. Sundholm, F. Cossio, M. A. Petrukhina, J. Wu, J. Wu, A. Restrepo, *Chem. Sci.*, 2023, 14, 5569-5576. (The questions that were sent out to the participants were prepared by **Miquel Sola and I**)
- 64- Metallaaromaticity – A Protean World. B. J. R. Cuyacot, Z. Badri, A. Ghosh\*, **C. Foroutan-Nejad\***, *Phys. Chem. Chem. Phys.*, 2022, 24, 27957-27963.
- 63- Reductive Elimination from Sterically Encumbered Ni–Polypyridine Complexes. C. S. Day, S. J. Ton, R. T. McGuire, **C. Foroutan-Nejad\***, R. Martin\*, *Organometallics*, 2022, 19, 2662-2667.
- 62- Cationic Gold (II) Complexes: Experimental and Theoretical Study. J. Mehara, A. K. Surendran, T. v. Wieringen, D. Setia, **C. Foroutan-Nejad**, M. Straka, L. Rulíšek, J. Roithová\*, *Chem. Eur. J.*, 2022, e202201794.

- 61- Room-Temperature-Stable Magnesium Electride via Ni (II) Reduction. C. S. Day, C. D. Do, C. Odena, J. Benet-Buchholz, L. Xu, **C. Foroutan-Nejad\***, K. H. Hopmann\*, R. Martin\*, **J. Am. Chem. Soc.** 2022, 144, 13109-13117.
- 60- On-Surface Azide–Alkyne Cycloaddition Reaction: Does It Click with Ruthenium Catalysts? T. Li, E. M. Dief, Z. Kalužná, M. MacGregor, **C. Forouatan-Nejad\***, N. Darwish\*, **Langmuir**, 2022, 38, 5532-5541.
- 59- Collective interactions among organometallics are exotic bonds hidden on lab shelves. S. Sowlati-Hashjin, V. Šadek, S. A. Sadjadi, M. Karttunen, A. Martín-Pendás\*, **C. Forouatan-Nejad\***, **Nat. Commun.** 2022, 13, 2069.
- 58-  $[\{\text{Th}(\text{C}_8\text{H}_8)\text{Cl}_2\}_3]^{2-}$  Is Stable but Not Aromatic. B. J. R. Cuyacot, **C. Forouatan-Nejad\***, **Nature**, 2022, 603, E18-E20.
- 57- Path-Dependency of Energy Decomposition Analysis & the Elusive Nature of Bonding. J. Poater\*, D. M. Andrada\*, M. Sola\*, **C. Foroutan-Nejad\***, **Phys. Chem. Chem. Phys.** 2022, 24, 2344-2348.
- 56- A double bond with weak sigma- and strong pi-interactions is still a double bond. **C. Foroutan-Nejad\***, **Nat. Commun.** 2021, 12, 4037.
- 55- Bonding and Aromaticity in Electron-Rich Boron and Aluminum Clusters. **C. Foroutan-Nejad\***, **J. Phys. Chem. A** 2021, 125, 6, 1367–1373. (Invited Paper; the A. I. Boldyrev's Festschrift).
- 54- Anatomy of Base Pairing in DNA by Interacting Quantum Atoms. B. J. R. Cuyacot, I. Durnik, C. Foroutan-Nejad\*, R. Marek\*, **J. Chem. Inf. Model.** 2021, 61, 1, 211–222.
- 53- Energy components in energy decomposition analysis (EDA) are path functions; why does it matter? D. M. Andrada\*, **C. Foroutan-Nejad\***, **Phys. Chem. Chem. Phys.** 2020, 22, 22459-22464.
- 52- From  $\pi$  Bonds without  $\sigma$  Bonds to the Longest Metal–Metal Bond Ever: A Survey on Actinide–Actinide Bonding in Fullerenes. A. Jaroš, **C. Foroutan-Nejad\***, M. Straka\*, **Inorg. Chem.** 2020, 59, 12608-12615.
- 51- Na...B Bond in  $\text{NaBH}_3^-$ ; A Different Type of Bond. **C. Foroutan-Nejad\***, **Angew. Chem. Int. Ed.** 2020, 59, 20900-20903.
- 50- Relativity or Aromaticity? A First-Principles Perspective of Chemical Shifts in Osmabenzene and Osmapentalene Derivatives. **C. Foroutan-Nejad\***, J. Vicha, A\*. Ghosh\*, **Phys. Chem. Chem. Phys.** 2020, 22, 10863-10869.
- 49- Fullerene-Based Switching Molecular Diodes Controlled by Oriented External Electric Fields. A. Jaroš, E. F. Bonab, M. Straka\*, **C. Foroutan-Nejad\***, **J. Am. Chem. Soc.** 2019, 141, 19644-19654.
- 48- Bifurcated hydrogen bonds in platinum(II) complexes with phosphinoamine ligands. M. Sojka, J. Tousek, Z. Badri, **C. Foroutan-Nejad**, M. Necas\*, **Polyhedron** 2019, 170, 593-601.
- 47-  $^1\text{H-NMR}$  is not a proof of hydrogen bonds in transition metal complexes. J. Vicha\*, **C. Foroutan-Nejad\***, M. Straka\*, **Nat. Commun.** 2019, 10, 1643.

- 46- Norcorrole as a delocalized antiaromatic system. J. Conradie\*, **C. Foroutan-Nejad\***, A. Ghosh\*, **Sci. Rep.** 2019, 9, 4852.
- 45- Electrochemical metallization ReRAMs (ECM) - Experiments and modelling: general discussion. E. Ambrosi, P. Bartlett, S. Berg, S. Brivio, G. Burr, S. Deswal, J. Deuermeier, M. Haga, A. Kiazadeh, G. Kissling, M. Kozicki, **C. Foroutan-Nejad**, E. Gale, Y. Gonzalez-Velo, A. Goossens, L. Goux, T. Hasegawa, H. Hilgenkamp, R. Huang, S. Ibrahim, D. Ielmini, T. Kenyon, V. Kolosov, Y. Li, S. Majumdar, G. Milano, T. Prodromakis, N. Raeishosseini, V. Rana, C. Ricciardi, M. Santamaria, A. Shluger, I. Valov, R. Waser, S. Williams, D. Wouters, Y. Yang, A. Zaffora, **Faraday Discuss.** 2019, 213, 115-120.
- 44- Phase-change memories (PCM) Experiments and modelling: general discussion. P. Bartlett, M. Bernasconi, S. Brown, G. Burr, **C. Foroutan-Nejad**, E. Gale, R. Huang, D. Ielmini, G. Kissling, V. Kolosov, M. Kozicki, H. Nakamura, K. Rushchanskii, M. Salinga, A. Shluger, D. Thompson, I. Valov, W. Wang, R. Waser, S. Williams, **Faraday Discuss.** 2019, 213, 393-420.
- 43- Magnetic Diversity in Heteroisocorroles: Aromatic Pathways in 10-Heteroatom-Substituted Isocorroles. **C. Foroutan-Nejad\***, A. Ghosh\*, **ACS Omega**, 2018, 3, 15865.
- 42- Local: Versus global aromaticity in azuliporphyrin and benziporphyrin derivatives. A. Ghosh\*, S. Larsen, J. Conradie, **C. Foroutan-Nejad\***, **Org. Biomol. Chem.** 2018, 16, 7964.
- 41- Buckyball Difluoride  $F_2@C_{60}^+$ ; a Single-Molecule Crystal. **C. Foroutan-Nejad\***, M. Straka\*, I. Fernandez\*, G. Frenking\*, **Angew. Chem. Int. Ed.** 2018, 57, 13931/**Angew. Chem.** 2018, 130, 14127.
- 40- Isocorroles as Homoaromatic NIR-Absorbing Chromophores: A First Quantum Chemical Study. **C. Foroutan-Nejad\***, S. Larsen, J. Conradie, A. Ghosh\*, **Sci. Rep.** 2018, 8, 11952.
- 39- Why Is Benzene Unique? Screening Magnetic Properties of  $C_6H_6$  Isomers. T. Janda, **C. Foroutan-Nejad\***, **ChemPhysChem** 2018, 19, 2357-2363.
- 38- How Does a Container Affect Acidity of its Content: Charge-Depletion Bonding Inside Fullerenes. A. Jaroš Z. Badri, P. Lochan Bora, E. Farajpour Bonab, R. Marek, M. Straka\*, **C. Foroutan-Nejad\***, **Chem. Eur. J.** 2018, 24, 4245-4249.
- 37- Nature of three electron bonds. D. Danovich\*, **C. Foroutan-Nejad\***, Philippe Hiberty\*, Sason Shaik\*, **J. Phys. Chem. A** 2018, 122, 1873-1885 (**Invited Paper; virtual special issue Manuel Yáñez and Otilia Mó Festschrift**).
- 36- Anti-Electrostatic CH-Ion Bonding in Decorated Graphanes. M. Novák, R. Marek, **C. Foroutan-Nejad\*** **Chem. Eur. J.** 2017, 23, 14931-14936.
- 35- Supramolecular Covalence in Bifurcated Chalcogen Bonding. P. L. Bora, M. Novák, J. Novotný, **C. Foroutan-Nejad**, R. Marek\* **Chem. Eur. J.** 2017, 23, 7315–7323.



- 34- Aromaticity, the Huckel  $4n + 2$  Rule and Magnetic Current. L. Zhao, R. Grande-Aztatzi, **C. Foroutan-Nejad\***, J. M. Ugalde\*, G. Frenking\*, **ChemistrySelect** 2017, 2, 863-870.
- 33- Dipolar molecules inside C 70: an electric field-driven room-temperature single-molecule switch. **C. Foroutan-Nejad\***, V. Andrushchenko, M. Straka\*, **Phys. Chem. Chem. Phys.** 2016, 18, 32673-32677.
- 32- Solvent effects on ion–receptor interactions in the presence of an external electric field. M. Novák, **C. Foroutan-Nejad\***, R. Marek, **Phys. Chem. Chem. Phys.** 2016, 18, 30754-30760.
- 31- Modulating Electron Sharing in Ion- $\pi$ -Receptors via Substitution and External Electric Field: A Route toward Bond Strengthening. M. Novák, **C. Foroutan-Nejad\***, R. Marek, **J. Chem. Theory Comput.** 2016, 12, 3788-3795.
- 30- Unification of Ground-State Aromaticity Criteria –Structure, Electron Delocalization, and Energy– in the Light of the Quantum Chemical Topology. Z. Badri, **C. Foroutan-Nejad\***, **Phys. Chem. Chem. Phys.** 2016, 18, 11693-11699 (**Invited Paper; Special Issue on Electron delocalization and aromaticity: 150 years of the Kekulé benzene structure**).
- 29- Multicenter Covalency: Revisiting the Nature of Anion- $\pi$  Interactions. **C. Foroutan-Nejad\***, Z. Badri, R. Marek\*, **Phys. Chem. Chem. Phys.** 2015, 17, 30670-30679.
- 28- On the Non-Classical Contribution in Lone Pair- $\pi$  Interaction: IQA perspective. Z. Badri\*, **C. Foroutan-Nejad\***, J. Kozelka, R. Marek\*, **Phys. Chem. Chem. Phys.** 2015, 17, 26183-26190.
- 27- Unwilling U–U Bonding in U2@ C80. Cage-Driven Metal Metal Bonds in Di-Uranium Fullerenes. **C. Foroutan-Nejad\***, J. Vícha, R. Marek, M. Patzschke, M. Straka\*, **Phys. Chem. Chem. Phys.** 2015, 17, 24182-24192.
- 26- Understanding the Electronic Factors Responsible for Ligand Spin–Orbit NMR Shielding in Transition-Metal Complexes. J. Vícha, **Cina Foroutan-Nejad\***, T. Pawlak, M. L. Munzarová, M. Straka\*, R. Marek\*, **J. Chem. Theory Comput.** 2015, 11, 1509-1517.
- 25- Comment on “Some Unexpected Behavior of the Adsorption of Alkali Metal Ions onto the Graphene Surface under the Effect of External Electric Field”. **C. Foroutan-Nejad\***, M. Novák, R. Marek, **J. Phys. Chem. C** 2015, 119, 5752-5754.
- 24- Asymmetric bifurcated halogen bonds. Martin Novák, **C. Foroutan-Nejad\***, R. Marek\*, **Phys. Chem. Chem. Phys.** 2015, 17, 6440-6450.
- 23- Is NICS a reliable aromaticity index for transition metal clusters? **C. Foroutan-Nejad\***, **Theor. Chem. Acc.** 2015, 134, 1-9. (**Topical Collection XI Girona Seminar Collection: Carbon, Metal, and Carbon-Metal Clusters**).
- 22- Design of Stereo–Electronically Promoted Super–Lewis Acids and Unprecedented Chemistry of Their Complexes. **C. Foroutan-Nejad\***, J. Vícha, R. Marek\*, **Chem. Eur. J.** 2014, 20, 11584-11590.



- 21-** Toward a consistent interpretation of the QTAIM: Tortuous link between chemical bonds, interactions and bond/line paths. **C. Foroutan-Nejad**, S. Shahbazian, R. Marek, **Chem. Eur. J.** 2014, 20, 10140-10152. **(Highly Cited Paper, June to September 2015 According to ISI Web of Knowledge).**
- 20-** The Origin of Thermodynamic Stability of Polymorph IV of Crystalline Barbituric Acid: Evidences from Solid-State NMR and Electron Density Analyses. Z. Badri, K. Bouzková, **C. Foroutan-Nejad**, R. Marek\*, **Cryst. Growth Des.** 2014, 14, 2763-2772.
- 19-** Potential energy surface and binding energy in the presence of an external electric field: modulation of anion- $\pi$  interactions for graphene-based receptors. **C. Foroutan-Nejad\***, R. Marek\*, **Phys. Chem. Chem. Phys.** 2014, 16, 2508-2514.
- 18-** All-metal aromaticity: revisiting the ring current model among transition metal clusters. Z. Badri, S. Pathak, H. Fliegl, P. Rashidi-Ranjbar, R. Bast, R. Marek, **C. Foroutan-Nejad\***, K. Ruud\*, **J. Chem. Theory Comput.** 2013, 9, 4789-4796.
- 17-** A theoretical survey on the  $D_{7d}$  [84]fullerene, a fullerene with two heptagon rings. Z. Badri, **C. Foroutan-Nejad**, P. Rashidi-Ranjbar\*, **Comput. Theor. Chem.** 2013, 1009, 103-107.
- 16-**  $Al_4^{2-}$ ; the anion- $\pi$  interactions and aromaticity in the presence of counter ions. **C. Foroutan-Nejad\***, **Phys. Chem. Chem. Phys.** 2012, 14, 9738-9748.
- 15-** Method/basis set dependence of NICS values among metallic nano-clusters and hydrocarbons. Z. Badri, **C. Foroutan-Nejad\***, P. Rashidi-Ranjbar\*, **Phys. Chem. Chem. Phys.** 2012, 14, 3471-3481.
- 14-** Molecular structure and antimicrobial activity of binuclear Ag (I) complex of phenyl bis(2-pyridyl)phosphine. A. Nemat Kharat\*, A. Bakhoda, S. Foroutan-Nejad, **C. Foroutan-Nejad**, **Zeitschrift für anorganische und allgemeine Chemie**, 2011, 637, 2260-2264.
- 13-** Laplacian of electron density vs. NICS<sub>zz</sub> scan: measuring magnetic aromaticity among molecules with different atom types. **C. Foroutan-Nejad**, Z. Badri, S. Shahbazian, P. Rashidi-Ranjbar\*, **J. Phys. Chem. A** 2011, 115, 12708-12714. **(Invited Paper; the R. F. W. Bader's Festschrift).**
- 12-** Inter-Atomic Magnetizability: a QTAIM-Based Approach toward Deciphering Magnetic Aromaticity. **C. Foroutan-Nejad\***, **J. Phys. Chem. A** 2011, 115, 12555-12560. **(Invited Paper; the R. F. W. Bader's Festschrift).**
- 11-** How Electron Delocalization Affect the Electronic Energy? A Survey among Neutral Poly-Nitrogen Clusters. J. Najafpour\*, **C. Foroutan-Nejad**, H. Shafiee, M. Kordi Peykani, **Comput. Theor. Chem.** 2011, 974, 86-91.
- 10-** Reply to "Is there a connection between electron densities at the ring critical points and NICS? A comment on "The electron density vs. NICS scan: a new approach to assess aromaticity in molecules with different ring sizes." **C. Foroutan-Nejad\***, S. Shahbazian\*, P. Rashidi-Ranjbar\*, **Phys. Chem. Chem. Phys.** 2011, 13, 12655-12658.

- 9- A Dissected Ring Current Model for Assessing Magnetic Aromaticity: A General Approach for both Organic and Inorganic Rings. **C. Foroutan-Nejad**, S. Shahbazian, Ferran Feixas, P. Rashidi-Ranjbar\*, Miquel Sola\*, **J. Comput. Chem.** 2011, 32, 2422-2431.
- 8- The Critical Re-evaluation of the Aromatic/Anti-aromatic Nature of  $Ti_3(CO)_3$ : A Missed Opportunity. **C. Foroutan-Nejad\***, S. Shahbazian\*, P. Rashidi-Ranjbar\*, **Phys. Chem. Chem. Phys.** 2011, 13, 4576-4582.
- 7- The Electron Density vs. NICS Scan: A New Approach to Assess Aromaticity in Molecules with Different Ring Sizes. **C. Foroutan-Nejad\***, S. Shahbazian\*, P. Rashidi-Ranjbar\*, **Phys. Chem. Chem. Phys.** 2010, 12, 12630-12637.
- 6- Topological characteristics of the Ring Critical Points and the aromaticity of groups IIIA to VIA heterobenzenes. A. A. Ebrahimi, R. Ghiasi, **C. Foroutan-Nejad\***, **J. of Mol. Struct. THEOCHEM** 2010, 941, 47-52.
- 5- Chemical bonding in the lightest tri-atomic clusters;  $H_3^+$ ,  $Li_3^+$  and  $B_3^-$ . **C. Foroutan-Nejad**, P. Rashidi-Ranjbar\*, **J. of Mol. Struct. THEOCHEM** 2009, 901, 243-248.
- 4- Atomic basins with more than a single nucleus: A computational fact or a mathematical artifact? **C. Foroutan-Nejad\***, S. Shahbazian\*, **J. of Mol. Struct. THEOCHEM** 2009, 894, 20-22.
- 3- Application of quantum theory of atoms in molecules on small single wall (6, 0) zigzag carbon clusters. Part I: Topological analysis of electron density, structure and bonding. P. Rashidi-Ranjbar\*, A. Sadjadi, G. H. Shafiee, **C. Foroutan-Nejad**, **J. of Mol. Struct. THEOCHEM** 2008, 856, 79-87.
- 2- Facile and efficient pinacol rearrangement using tungstophosphoric acid ( $H_3PW_{12}O_{40}$ ) under solvent-free conditions. M. Yahyae, E. Kianmehr\*, **C. Foroutan-Nejad**, S. Beheshti, **B. Korean Chem. Soc.** 2006, 8, 1246-1248.
- 1- Ab initio charge density analysis of  $(B_6C)_2^-$  and  $B_4C_3$  species - How to describe the bonding pattern? **C. Foroutan-Nejad**, G. H. Shafiee, A. Sadjadi, S. Shahbazian\*, **Can. J. Chem.** 2006, 84, 771-781.

## 11. List of Publications Not Listed on the Web of Science

- 1- Principles of Molecular Devices Operated by Electric Fields. N. Darwish, **C. Foroutan-Nejad**, L. Domulevicz, J. Hihath, I. Díez-Pérez in "Effects of Electric Fields on Structure and Reactivity"; **New Horizons of Chemistry by Royal Society of Chemistry. (Invited Book Chapter)**

## 12. Selected Invited Talks and Chairing Conferences

- 17- Illusive carbon-carbon ylides. **International Conference on Chemical Bonding (ICCB 2016)**, 23-28 August 2025, Organized by **University of California Los Angeles-UCLA at Kauai, Hawaii, U.S.A.**

- 16- Modern Chemical Bond Theories, 11-14 February 2024 Arctic University of Norway, Tromso, Norway
- 15- Designing Organic Electronics, 11-14 February 2024 Arctic University of Norway, Tromso, Norway
- 14- Why Should We Be Worried About Path-Dependency of EDA? **International Conference on Noncovalent Interactions (ICNI)**, 18-22 July 2022, Strasbourg, France.
- 13- From Memristor to Spinristor; Endohedral Metallofullerenes for Molecular Electronics **10<sup>th</sup> International Conference on Molecular Electronics (ElecMol)**, 29 November-2 December 2021, Lyon, France.
- 12- Ground and excited state aromaticity, **International Conference on Excited-State Aromaticity and Antiaromaticity, ICESAA 1**, 29 July-2 August 2019, Upsala University, Sigtuna, Sweden.
- 11- The perspective of energy consumption in a digital world, **URBIS SMART CITY FAIR**, 5-6 June 2019, Brno, Czechia.
- 10- Molecular memories, **XII Summer School of Chemistry**, 12-13 September 2018, Masaryk University, Brno, Czechia.
- 9- A series of talks on Chemical Bond Theory in Annual Workshop of Modern Methods in Quantum Chemistry, Mariapfarr Austria (2013 – 2017 and 2023)
- 8- Manipulating Inter-Molecular Interactions via External Fields, Invited talk for the theoretical chemistry group, 16-18 November 2016, **Philipps Universitat Marburg, Marburg, Germany**.
- 7- Unification of Ground-State Aromaticity Criteria, **International Symposium on Theoretical Chemical Physics, ISTCP IX**, 17-22 July 2016, Grand Forks, North Dakota, U.S.A.
- 6- Chairing the chemical concept session of **International Symposium on Theoretical Chemical Physics, ISTCP IX on Chemical Concepts**, 17-22 July 2016, Grand Forks, North Dakota, U.S.A.
- 5- Manipulating Inter-Molecular Interactions via External Fields, **International Conference on Chemical Bonding (ICCB 2016)**, 14-18 July 2016, Organized by University of California Los Angeles-UCLA at Kauai, Hawaii, U.S.A.
- 4- In Silico Design and Chemistry of Stereo-Electronically Promoted Super Lewis Acids, **Summer Symposium of the Amsterdam Center for Multiscale Modeling (ACMM)**, 25 June 2015, Amsterdam, Netherlands.

**3- Chairing the theoretical/computational session of 30th Central European NMR Meeting, 19.4-22.4.2015, Valtice, Czech Republic.**

**2- All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters, Workshop on Magnetically Induced Currents in Molecules, 17-21 November 2014, Tvarminne, Finland.**

**1- Aromaticity from NICS to Bond Magnetizability, C. Foroutan-Nejad, Changsha International Quantum Chemistry Workshop, 7-8 June 2012, Changsha, China.**