Cina Foroutan-Nejad

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Publon URL: https://publons.com/researcher/906865/cina-foroutan-nejad/
Number of ISI Journal Publications:
55 (**4** in **2016**, **3** in **2017**, **7** in **2018**, **6** in **2019**, **4** in **2020,** and **2** in **2021**)
Corresponding author in **37 publications**
Number of **Single-Author Publications**: **5**
Number of **Invited Papers**: **5 (4** by **American Chemical Society, 2** by **Royal Society of Chemistry)**
Full list of publications available at:
https://scholar.google.cz/citations?user=tc6ZQV4AAAAJ&hl=en
Invited Talks: **9 (1** in **2012**, **1** in **2014**, **1** in **2015**, **3** in **2016, 1** in **2018**, and **1 in 2019**)
H-Index: **20 (WoS) / 20 (Scopus) / 21 (Google Scholar)**
Number of Citations: **1120 and counting (WoS)**
H-Index limited to publications in past **3 years (2018-2021)**: **7 (WoS)**
Supervisor/Advisor of **6** theses (**5** PhD, **1** MS, and **1** BSc)

Education and Training

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-cyclopropa [e] pyrene: a mechanistic study
Specialization Reaction Mechanisms and Computational Chemistry

1998–2002 B.Sc. in Applied Chemistry
Azad University, Tehran, Central Branch

Research Interests and Experience

Molecular Electronics: Fullerene-Based Electronics, Field-Effect on Chemical Processes, Mono-Molecular Memristors
Chemical Bond Theory: Quantum Theory of Atoms in Molecules, Supramolecular Chemistry, Charge-Transfer Processes, Aromaticity
Magnetic Response Properties: Current Density Analysis, Relativistic Effects in NMR
Catalysis: Designing Super-Lewis Acids

Current Collaborations

Prof. **Abhik Ghosh** (Arctic University of Norway-University of Tromsø, Tromsø, Norway) **Magnetic Response Properties, Aromaticity**

Doc. **Michal Straka** (IOCB, Prague, Czech Republic) **Molecular Electronics; Theoretical Aspects**

Dr. Simone Ciampi & Dr. Nadim Darwish (Curtin University, Perth, Australia) **Molecular Electronics; Experimental Aspects**

Past Collaborations

Prof. **Sason Shaik** (Hebrew University of Jerusalem, Jerusalem, Israel)

Prof. **Gernot Frenking** (Philipps-Universitat Marburg, Marburg, Germany)

Prof. **Kenneth Ruud** (Arctic University of Norway-University of Tromsø, Tromsø, Norway)

Prof. **Miquel Solà** (University of Girona, Girona, Spain)

Research Funding

2018-2019 420,000 CZK, GAMU E, Prize for excellent results

2017-2020 3,615,000 CZK, Ministry of Education, Czech Republic (GACR) (36 Months)

September 2014 2,000 € Award from Center of Theoretical and Computational Chemistry (CTCC), Norway, for covering research stay in Norway

2014-2017 129,558 € Marie Curie Fellowship (26 Months)

Reviewing Activity

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

Reviewer of **Journal of the American Chemical Society**, **Angewandte Chemie**, **Nature Communications**, **Chemical Communications**, **Chemistry-A European Journal**, and many more.

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

Full list of reviewing activity is available at Publons:

https://publons.com/author/906865/cina-foroutan-nejad#profile

Honors and Awards

2003	Ranked 8 among 10,000+ applicants for Unified Entrance Exam of Master degree in Chemistry.
2006	Ranked 1st for PhD entrance exam of chemistry among 200+ applicants
2003-2010	Top student of the University of Tehran
2012	2-years honorary membership of Royal Society of Chemistry for my contribution in physical chemistry as a young researcher

Publications

- The asterisks (*) denote those publications that I have been their contact author.
- The number of citations in ISI journals are presented in parenthesis in the end of each publication.

55- Bonding and Aromaticity in Electron-Rich Boron and Aluminum Clusters. **C. Foroutan-Nejad***, *J. Phys. Chem. A* **2021**, DOI: 10.1021/acs.jpca.0c11474 (*Invited Paper for Alexander Boldyrev festschrift*)

54- Anatomy of Base Pairing in DNA by Interacting Quantum Atoms. B. J. R. Cuyacot, I Durník, **C. Foroutan-Nejad***, Radek Marek, *J. Chem. Inf. Model.* **2021**, 211-222.

53- Energy components in energy decomposition analysis (EDA) are path functions; why does it matter? D. Andrada, **C. Foroutan-Nejad***, *Phys. Chem. Chem. Phys.* **2020**, 22, 22459-22464. (4)

52- From π Bonds without σ Bonds to the Longest Metal-Metal Bond Ever: A Survey on Actinide-Actinide Bonding in Fullerenes. A. Jaros, **C.Foroutan-Nejad***, M. Straka, *Inorg. Chem.* **2020**, 59, 12608-12615. (1)

51- Na…B Bond in $NaBH_3^-$; A Different Type of Bond. **C. Foroutan-Nejad***, *Angew. Chem. Int. Ed.* **2020**, 59, 20900-20903. (2)

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. (2)

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. (21)

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. (2)

47- ^{1}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. (6)

46- Norcorrole as a delocalized antiaromatic system. J. Conradie, **C. Foroutan-Nejad***, A. Ghosh, *Sci. Rep.* **2019**, 9, 4852. (7)

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. (3)

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. (2)

43- Magnetic Diversity in Heteroisocorroles: Aromatic Pathways in 10-Heteroatom-Substituted Isocorroles. **C. Foroutan-Nejad***, A. Ghosh, *ACS Omega*, **2018**, 3, 15865. (7)

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. (7)

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. **(**VIP paper; 12**)**

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. (8)

39- Why Is Benzene Unique? Screening Magnetic Properties of C6H6 Isomers. T. Janda, **C. Foroutan-Nejad***, *ChemPhysChem* **2018**, 19, 2357-2363. (11)

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. (14)

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*). (11)

36- Anti-Electrostatic CH-Ion Bonding in Decorated Graphanes. M. Novák, R. Marek, **C. Foroutan-Nejad*** *Chem. Eur. J.* **2017**, 23, 14931-14936. (7)

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. (28)

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. (36)

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. (31)

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. (10)

31- Modulating Electron Sharing in Ion-π-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. (24)

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*) (41)

29- Multicenter Covalency: Revisiting the Nature of Anion-π Interactions. **C. Foroutan-Nejad***, Z. Badri, R. Marek, *Phys. Chem. Chem. Phys.*, **2015**, 17, 30670-30679. (55)

28- On the Non-Classical Contribution in Lone Pair-π Interaction: IQA perspective. Z. Badri, **C. Foroutan-Nejad**, J. Kozelka, R. Marek, *Phys. Chem. Chem. Phys.*, **2015**, 17, 26183-26190. (42)

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)

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. (41)

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. (14)

24- Asymmetric bifurcated halogen bonds. Martin Novák, **C. Foroutan-Nejad***, R. Marek, *Phys. Chem. Chem. Phys.* **2015**, 17, 6440-6450. (37)

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*) (45)

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. (9)

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*) (145)

20- 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. (18)

19-Potential energy surface and binding energy in the presence of an external electric field: modulation of anion–π interactions for graphene-based receptors. **C. Foroutan-Nejad***, R. Marek, *Phys. Chem. Chem. Phys.* **2014**, 16, 2508-2514. (29)

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. (59)

17- A theoretical survey on the D7d [84]fullerene, a fullerene with two heptagon rings. Z. Badri, **C. Foroutan-Nejad**, P. Rashidi-Ranjbar, *Comput. Theor. Chem.* **2013**, 1009, 103-107. (4)

16- Al_4^{2-}; the anion–π interactions and aromaticity in the presence of counter ions. **C. Foroutan-Nejad***, *Phys. Chem. Chem. Phys.* **2012**, 14, 9738-9748. (12)

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. (11)

14- Molecular structure and antimicrobial activity of binuclear Ag (I) complex of phenyl bis(2-pyridyl)phosphine. A. Nemati Kharat A. Bakhoda, S. Foroutan-Nejad, **C. Foroutan-Nejad**, *Zeitschrift für anorganische und allgemeine Chemie*, **2011**, 637, 2260-2264. (13)

13- Laplacian of electron density *vs.* $NICS_{zz}$ 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*) (23)

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*) (35)

11- How Does 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. (19)

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. (14)

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. (39)

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. (24)

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. (52)

6- Topological characteristics of the Ring Critical Points and the aromaticity of groups IIIA to VIA hetero-benzenes. A. A. Ebrahimi, R. Ghiasi, **C. Foroutan-Nejad***, *Journal of Molecular Structure: THEOCHEM*, **2010**, 941, 47-52. (31)

5- Chemical bonding in the lightest tri-atomic clusters; H_3^+, Li_3^+ and B_3^-. **C. Foroutan-Nejad**, P. Rashidi-Ranjbar, *Journal of Molecular Structure: THEOCHEM*, **2009**, 901, 243-248. (13)

4- Atomic basins with more than a single nucleus: A computational fact or a mathematical artifact? **C. Foroutan-Nejad***, S. Shahbazian, *Journal of Molecular Structure: THEOCHEM*, **2009**, 894, 20-22. (14)

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**, *Journal of Molecular Structure: THEOCHEM*, **2008**, 856, 79-87. (4)

2- Facile and efficient pinacol rearrangement using tungstophosphoric acid ($H_3PW_{12}O_{40}$) under solvent-free conditions. M. Yahyaee, E. Kianmehr, **C. Foroutan-Nejad**, S. Beheshti, *Bulletin of the Korean Chemical Society*, **2006**, 8, 1246-1248. (4)

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, *Candian Journal of Chemistry*, **2006**, 84, 771-781. (17)

Invited Talks and Chairing Conferences

10- Ground and excited state aromaticity, **ICESSA 1**, 29 July-2 August, **2019**, Upsala University, Sweden.

9- Molecular memories, XII Summer School of Chemistry, 12-13 September **2018**, Masaryk University

8- *Manipulating Inter-Molecular Interactions via External Fields*, 16-18 November, **2016**, Philipps Universitat Marburg, Marburg, Germany. Invited talk for the theoretical chemistry group.

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 Workshop, 7-8 June, **2012**, Changsha, China.