

IN THE NAME OF GOD

Curriculum Vitae

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Research Activity

Quantum calculations

2-D carbon structures: Graphene, Graphyne and Graphdiyne

Hydrogen storage

Adsorption

Theoretical study of the kinetic and thermodynamic properties of reactions

Nanostructures

Theoretical investigation of nanostructures

Aromaticity and anti-aromaticity of compounds

Education

1993-1997, Bachelor of Chemistry, Isfahan University, Isfahan, Iran.

1997-1999, Master of science in Physical Chemistry, Iran University of Science &
Technology, Tehran, Iran.

2004-2009, Ph.D. of Physical Chemistry, University of Kashan, Kashan, Iran.

Teaching Experiences

1. General Chemistry (I)

2. Physical Chemistry (I)
3. Physical Chemistry (II)
4. Laboratory of Physical Chemistry (I) & (II)
5. Quantum Chemistry (I)
6. Quantum Chemistry (II) (M.Sc.)
7. Molecular Spectroscopy (I)
8. Advance Physical Chemistry (M.Sc.)
9. New Topics in Physical Chemistry (Ph.D.)
10. Advance Chemical Kinetics
11. Computational Chemistry

Journal Publications:

1. F. Akbari, **A. Reisi-Vanani**, M.H. Darvishnejad, DFT study of the electronic and structural properties of single Al and N atoms and Al-N co-doped graphyne toward hydrogen storage, *Applied Surface Science*, 488 (2019) 600-610.
2. F. Mofidi, **A. Reisi-Vanani**, Sensing and elimination of the hazardous materials such as Sarin by metal functionalized γ -graphyne surface: A DFT study, *Journal of Molecular Liquids*, 286 (2019) 110929.
3. Z. Mirzaie, **A. Reisi-Vanani**, M. Barati, Polyvinyl alcohol-sodium alginate blend, composited with 3D-graphene oxide as a controlled release system for curcumin, *Journal of Drug Delivery Science and Technology*, (2019).
4. M. Shams, **A. Reisi-Vanani**, Potassium decorated γ -graphyne as hydrogen storage medium: Structural and electronic properties, *International Journal of Hydrogen Energy*, 44 (2019) 4907-4918.
5. M. Ebadi, **A. Reisi-Vanani**, F. Houshmand, P. Amani, Calcium-decorated graphdiyne as a high hydrogen storage medium: Evaluation of the structural and electronic properties, *International Journal of Hydrogen Energy*, 43(52) (2018) 23346-23356.
6. S.K. Nasiri, **A. Reisi-Vanani**, M. Hamadani, Molecular Structure, Spectroscopic, Local and Global Reactivity Descriptors and NBO Analysis of C₃₂H₁₂: A New

Buckybowl and Sub-Fullerene Structure, Polycyclic Aromatic Compounds, (2018) *Impress*. <https://doi.org/10.1080/10406638.2018.1472108>

7. S.-D. Mousavi, F. Maghsoodi, F. Panahandeh, R. Yazdian-Robati, **A. Reisi-Vanani**, M. Tafaghodi, Doxorubicin delivery via magnetic nanomicelles comprising from reduction-responsive poly(ethylene glycol)-b-poly(ϵ -caprolactone) (PEG-SS-PCL) and loaded with superparamagnetic iron oxide (SPIO) nanoparticles: Preparation, characterization and simulation, *Materials Science and Engineering: C*, 92 (2018) 631-643.
8. F. Hajizadeh, **A. Reisi-Vanani**, Y.T. Azar, Theoretical design of Zn-dithiaporphyrins as sensitizer for dye-sensitized solar cells, *Current Applied Physics*, 18 (2018) 1122-1133.
9. A. Rezaei, **A. Reisi-Vanani**, S. Masoum, An Application of Geometrical Isometries in Nonplanar Molecules, *Iranian Journal of Mathematical Chemistry*, 9(4) (2018) 255-261.
۱۰. نرگس صائمی، مهدی شبانی نوش آبادی، سعید معصوم، عادل رئیسی وانانی، بررسی خواص بازدارندگی شیف بیس [۲- (فنیل تیو) بنزیلیدن] او ۴- فنیلن دی آمین بر خوردگی فولاد ۳۱۰ در محیط اسیدی با استفاده از طراحی آزمایش و محاسبات کوانتومی، فصل نامه علوم و مهندسی خوردگی، سال هفتم (۲۰۱۷) ۶۱-۷۳.
۱۱. عادل رئیسی وانانی، فاطمه حاجیزاده، بررسی خصلت آروماتیکی برخی نانوساختارهای کربنی پلی سیکلی کاسه ای شکل، شیمی کاربردی دانشگاه سمنان، ۴۴ (۲۰۱۷) ۱۰۹-۱۲۰.
12. **A. Reisi-Vanani**, F. Shamsali, Influence of nitrogen doping in sumanene framework toward hydrogen storage: A computational study, *Journal of Molecular Graphics and Modelling*, 76 (2017) 475-487.
13. **A. Reisi-Vanani**, Z. Shabani, Evaluation of the hydrogen adsorption onto Li and Li + decorated circumtrindene ($C_{36}H_{12}$): A theoretical study, *International Journal of Hydrogen Energy*, 42 (2017) 22973-22986.
14. **A. Reisi-Vanani**, M. Safipoor, Investigation of carbon monoxide adsorption onto sumanene ($C_{21}H_{12}$) decorated with Li^+ ions toward its elimination, *Current Applied Physics*, 17 (2017) 1382-1395.

15. A. Reisi-Vanani, S. Hoseinpour, A theoretical investigation of decomposition and reactivity of the atmospheric $C_3F_7OCH_2O$ radical, *Arabian Journal of Chemistry*, 10 (2017) S1604-S1612.
16. M. Afzalkhah, S. Masoum, M. Behpour, H. Naeimi, **A. Reisi-Vanani**, Experimental and Theoretical Investigation of Inhibition Efficiency of 2-(2-Hydroxyphenyl)-benzothiazole Using Impedance Spectroscopy, Experimental Design, and Quantum Chemical Calculations, *Industrial & Engineering Chemistry Research*, 56 (2017) 9035-9044.
17. **A. Reisi-Vanani**, S. Mehrdoust, Effect of boron doping in sumanene frame toward hydrogen physisorption: A theoretical study, *International Journal of Hydrogen Energy*, 41 (2016) 15254-15265.
18. **A. Reisi-Vanani**, M. Hamadani, S.N. Kokhdan, Functionalization of the sumanene by nitrous oxide: A mechanistic study, *Computational and Theoretical Chemistry*, 1082 (2016) 49-57.
19. **A. Reisi-Vanani**, M. Hamadani, S.N. Kokhdan, Comprehensive theoretical study of the phenyl azide addition onto armchair (5, 5) single wall carbon nanotube, *Computational and Theoretical Chemistry*, 1075 (2016) 38-46.
20. **A. Reisi-Vanani**, S. Faghieh, Nucleus-Independent Chemical Shift Criterion for Aromaticity in Some of the Corannulene Derivatives as Carbon Nanostructure: Effect of Substituent Groups on Aromaticity, *Polycyclic Aromatic Compounds*, 36 (2016) 120-131.
21. **A. Reisi-Vanani**, S. Bahramian, Diazomethane addition to sumanene as a subfullerene structure: A theoretical mechanistic study, *Computational and Theoretical Chemistry*, 1093 (2016) 40-47.
22. S. Nasiri Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Ab initio and TD-DFT study of the structural and spectroscopic properties of $C_{30}H_{10}$ as a new bucky bowl, *Fullerenes, Nanotubes and Carbon Nanostructures*, 24 (2016) 577-587.
23. S. Hoseinpour, **A. Reisi-Vanani**, A mechanistic study for decomposition and reactivity of the $C_4F_9OC_2H_4O$ radical derived from HFE-7200 between 200–400 K, *Progress in Reaction Kinetics and Mechanism*, (2016).

24. **A. Reisi-Vanani**, L. Shahrokh, S.N. Kokhdan, Theoretical study of the corannulene ozonolysis and evaluation of the various reaction paths, *Computational and Theoretical Chemistry*, 1051 (2015) 72-78.
25. **A. Reisi-Vanani**, A.A. Rezaei, Evaluation of the aromaticity of non-planar and bowl-shaped molecules by NICS criterion, *Journal of Molecular Graphics and Modelling*, 61 (2015) 85-88.
26. **A. Reisi-Vanani**, S. Rahimi, S.N. Kokhdan, H. Ebrahimpour-Komleh, Computational study of the gas phase reaction of hydrogen azide and corannulene: A DFT study, *Computational and Theoretical Chemistry*, 1070 (2015) 94-101.
27. **A. Reisi-Vanani**, S. Hoseinpour, A computational study of the mechanism and kinetics for gas-phase decomposition and reactivity of the C₄F₉OCH₂O radical between 200 and 400 K, *Progress in Reaction Kinetics and Mechanism*, 40 (2015) 59-68.
28. V. Jabbari, M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, D. Villagran, In,V-codoped TiO₂ nanocomposite prepared via a photochemical reduction technique as a novel high efficiency visible-light-driven nanophotocatalyst, *RSC Advances*, 5 (2015) 78128-78135.
29. M. Izadyar, N. Zavvar, M. Khavani, **A. Reisi-vanani**, Secondary Structure Effects on the Acidity of Histidine and Lysine-Based Peptides Model; A Theoretical Study, *Physical Chemistry Research*, 3 (2015) 67-77.
30. **A. Reisi-Vanani**, S. Faghieh, Computational study of the molecular hydrogen physisorption in some of the corannulene derivatives as a carbon nanostructure, *Journal of Saudi Chemical Society*, 18 (2014) 666-673.
31. **A. Reisi-Vanani**, L. Alihoseini, Evaluation of the Aromaticity of a Non-Planar Carbon Nano-Structure by Nucleus-Independent Chemical Shift Criterion: Aromaticity of the Nitrogen-Doped Corannulene, *Journal of Nanostructures*, 4 (2014) 153-159.
32. **A. Reisi-Vanani**, L. Alihoseini, Computational investigation of the adsorption of molecular hydrogen on the nitrogen-doped corannulene as a carbon nano-structure, *Surface Science*, 621 (2014) 146-151.

33. **A. Reisi-Vanani**, M. Izadyar, A theoretical study of the mechanism and kinetics of the thermal decomposition of carbamoyl azide, *Progress in Reaction Kinetics and Mechanism*, 38 (2013) 305-315.
34. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, V. Jabbari, Photodeposition-assisted synthesis of novel nanoparticulate In, S-codoped TiO₂ powders with high visible light-driven photocatalytic activity, *Applied Surface Science*, 285 (2013) 121-129.
35. M. Hamadani, A. Reisi-Vanani, M. Behpour, A. Esmaeily, Synthesis and characterization of Fe, S-codoped TiO₂ nanoparticles: Application in degradation of organic water pollutants, *Desalination*, 281 (2011) 319-324.
36. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Sol-gel preparation and characterization of Co/TiO₂ nanoparticles: application to the degradation of methyl orange, *Journal of the Iranian Chemical Society*, 7 (2010) S52-S58.
37. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Synthesis, characterization and effect of calcination temperature on phase transformation and photocatalytic activity of Cu, S-codoped TiO₂ nanoparticles, *Applied Surface Science*, 256 (2010) 1837-1844.
38. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Preparation and characterization of S-doped TiO₂ nanoparticles, effect of calcination temperature and evaluation of photocatalytic activity, *Materials Chemistry and Physics*, 116 (2009) 376-382.

Conference papers:

1. M. Ebadi, **A. Reisi-Vanani**, F. Houshmand, Electronic, Magnetic and Structural Properties of Calcium Decorated Carbon 2-D Structure (Graphdiyne), 7th International Conference on Nanostructures (ICNS7), Sharif University of Technology, 27 Feb-1 Mar 2018.
2. M. Shams-Ghamsari, **A. Reisi-Vanani**, DFT study of potassium decorated γ -graphyne: Electronic structure and optical properties, 20th Iranian Physical Chemistry Conference, University of Arak, 20-22 Aug 2017.
3. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, The structure and spectroscopic properties of C₃₀H₁₀ as a new bucky bowl: DFT and TD-DFT study, 2nd international

- conference on new research achievement in chemistry and chemical engineering, 5 May **2016**.
4. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Full analysis of $C_{32}H_{12}$ as a new bucky bowl and a sub-fullerene structure: A theoretical study, 2nd international conference on new research achievement in chemistry and chemical engineering, 5 May **2016**.
 5. **A. Reisi-Vanani**, F. Hajizadeh, Theoretical study of dithiaporphyrin as sensitizer for dye-sensitized solar cells application, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
 6. **A. Reisi-Vanani**, M. Safipour, Computational investigation of the adsorption of CO on the Li⁺-decorated sumanene, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
 7. **A. Reisi-Vanani**, Z. Shabani, Effect of Li and Li⁺ decorating in circumtrindene ($C_{36}H_{12}$) frame toward hydrogen adsorption: A theoretical study, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
 8. **A. Reisi-Vanani**, S. Bahramian, Theoretical study of the sumanene nanostructure functionalization by diazomethane in the gas phase using density functional theory, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
 9. **A. Reisi-Vanani**, S.N. Kokhdan, M. Hamadani, Computational study of the gas phase reaction of HNCO and sumanene: A DFT study, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
 10. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Investigation of the reaction mechanism of the phenyl azide addition onto armchair (5,5) single wall carbon nanotube: An ONIOM study, 18th Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
 11. **A. Reisi-Vanani**, S. Mehrdoust, Theoretical Study of the Hydrogen Adsorption on Sumanene Nanostructure and its Boron Doped Derivatives: A Density Functional Theory Study, 18th Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.

12. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Theoretical study on the mechanism of cycloaddition reaction of nitrous oxide onto sumanene nanostructure, 18th Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
13. **A. Reisi-Vanani**, F. Shamsali, Quantum Study of the Hydrogen Adsorption on Nitrogen-doped Sumanene Nanostructure: A DFT and MP2 Study, 18th Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
۱۴. مهدی شبانی نوش آبادی، سعید معصوم، عادل رئیسی وانانی، نرگس صائمی، بررسی خواص بازدارندگی از خوردگی باز شیف N',N - بیس [۲- (فنیل تیو) بنزیلیدن] ۱، ۴- فنیلن دی آمین با استفاده از طراحی آزمایش آماری، شانزدهمین کنگره ملی خوردگی، پژوهشگاه صنعت نفت، ۳ و ۴ آذر ۱۳۹۴.
15. S. Rahimi, **A. Reisi-Vanani**, Theoretical study of the 1,3- dipolar cycloaddition of hydrogen azide to corannulene nanostructure ,17th Iranian Physical Chemistry Conference, University of Khaje-nasire-toosi, 21-23 October **2014**.
16. S. Faghih, **A. Reisi-Vanani**, Computational study of hydrogen storage on corannulene and its hydroxyl derivatives, 20th Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
17. L. Alihoseini, **A. Reisi-Vanani**, Theoretical investigation of hydrogen storage in corannulene and its nitrogen derivatives, 20th Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
18. L. Shahrokh, **A. Reisi-Vanani**, Theoretical study of the kinetics of the reaction of hydroxyl radical with corannulene nanostructure, 20th Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
19. S. Hoseinpour, **A. Reisi-Vanani**, Maryam Shamshiri, Rationalization of two-step mechanism of functionalization of single-walled carbon nanotubes with aryl diazonium salts: Comparison of OH and CH₂CH₃ substituent groups, Seminar of calculation in nanotechnology, Azad University, Oloum darouee branch, 16 February **2013**.
20. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, Combining Sol-Gel and Hydrothermal Methods With Photodeposition Method to Prepare In/TiO₂

Nanoparticles, Iran-Belarus International Conference on Modern Applications of Nanotechnology (IBCN12), Minsk, Belarus, June 27-29, **2012**.

21. **A. Reisi-Vanani**, S. Hoseinpour, Theoretical studies of decomposition and reactivity of the $C_3F_7OCH_2O$, 15th Iranian Physical Chemistry Conference, University of Tehran, September 4-6, **2012**.
22. **A. Reisi-Vanani**, S. Hoseinpour, Ab initio studies on the reactivity and thermal decomposition of the CF_3OCH_2O radical, 15th Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 4-6, **2012**.
23. M. Hamadian, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, Study of photocatalytic behavior of photochemical doped TiO_2 nanoparticles with In-V synthesized by sol-gel and hydrothermal methods, Nanomaterials: Applications and Properties, Sumy, Ukraine, September 17-22, **2012**.
24. **A. Reisi-Vanani**, M. Hamadian, Enhancement of the photocatalytic activity of doped and co-doped TiO_2 nanoparticles by metal and non-metal atoms and phase transformation, 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, **2011**.
25. Z. Tavangar, M. Hamadian, **A. Reisi-vanani**, Effect of calcination temperature on Preparation, Characterization and evaluation of photocatalytic activity of Sulfur doped TiO_2 nanoparticles, 11th Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
26. M. Hamadian, **A. Reisi-vanani**, Synthesis, characterization and effect of calcinations temperature on phase transformation and photocatalytic activity of Cu,S-codoped TiO_2 nanoparticles, 11th Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
27. **A. Reisi-Vanani**, M. Hamadian, Sol-gel preparation of Cu,S-codoped TiO_2 nanoparticles and evaluation of phase transformation and photocatalytic activity, 13th Iranian Seminar of Physical Chemistry, Shiraz University, April **2010**.
28. **A. Reisi-Vanani**, M. Hamadian, Effect of calcination temperature on preparation, phase transformation and photocatalytic activity of S- TiO_2 nanoparticles, First Seminar of responsibility of basic science in Nanotechnology, Imam Hosein University, Tehran, December **2009**.

29. **A. Reisi-Vanani**, M. Hamadani, Preparation and characterization of Co-TiO₂ nanoparticles and optimize Co content to degradation of methyl orange under UV and Visible irradiation, First Seminar of responsibility of basic science in Nanotechnology, Imam Hosein University, Tehran, December **2009**.
30. **A. Reisi-Vanani**, M. Hamadani, Preparation and characterization of pure TiO₂ nanoparticles, doping with Co, S and Fe-S and evaluation of photocatalytic activity to degradation of methyl orange and methylene blue under UV and Visible irradiation, 6th Student Seminar of Nanotechnology, Shahid Beheshti University of Medical Sciences, Tehran, December **2009**.
31. M. Hamadani, **A. Reisi-Vanani**, Preparation and Characterization of Fe, S and Fe-S co-Doped TiO₂, Nanoparticles and Evaluation of Photocatalytic Activity, 10th Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2009**.