

IN THE NAME OF GOD

Curriculum Vitae

Dr. Adel Reisi-Vanani

Professor of Physical Chemistry

Corresponding address: Department of Physical Chemistry, Faculty of Chemistry,
University of Kashan, P.O. Box. 87317-51167, Kashan, I.R. Iran

E-mail: *areisi@kashanu.ac.ir*

Tel: (+98)31-55912358

Fax: (+98)31-55912397

Research activity

Quantum and DFT calculations of:

- 2D carbon structures: Graphene, Graphyne and Graphdiyne
- CO₂ capture and CO₂ reduction reaction
- Water splitting
- Hydrogen storage
- Adsorption and deletion of toxic materials
- Kinetics and thermodynamics properties of reactions
- Electronic and structural properties 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 (M.Sc.)

Journal Publications:

1. G. Jafari, **A. Reisi-Vanani**, Boosting the electrocatalytic performance of the single Fe/Co atom anchored on pristine and B/N doped 8-16-4 graphyne for overall water splitting, *International Journal of Hydrogen Energy*, 175 (2025) 151528.
2. G. Jafari, **A. Reisi-Vanani**, Single-atom catalyst anchoring on 8-16-4-graphyne nanosheet: An efficient electrocatalyst for overall water splitting, *International Journal of Hydrogen Energy*, 109 (2025) 424-435.
3. A. Masiha, **A. Reisi-Vanani**, DFT study of the electrochemical CO₂ reduction by Sc to Ni single atom catalysts implanted on the pristine and N-doped-H_{4,4,4}-graphyne, *Fuel*, 372 (2024) 132225.
4. G. Jafari, **A. Reisi-Vanani**, Z. Tabandeh, Evaluation of the structural, electronic and magnetic properties of modified 8-16-4 graphyne by 3d transition metals: A DFT-D2 study, *Diamond and Related Materials*, 142 (2024) 110836.
5. M. Dehkhodaei, **A. Reisi-Vanani**, M. Sedghi, Computational investigation of charge injection into modified graphdiyne nanosheet via Al doping and Li decoration to improve hydrogen adsorption, *International Journal of Hydrogen Energy*, 64 (2024) 349-359.
6. A. Masiha, **A. Reisi-Vanani**, M. Hossein Darvishnejad, Evaluation of the CO₂ reduction reaction using Mn and Cr single atom catalysts implanted on the g-C₃N₄

(heptazine): A DFT study, *Computational and Theoretical Chemistry*, 1234 (2024) 114540

7. A. Meftahi, M. Shabani-Nooshabadi, **A. Reisi-Vanani**, Introducing GO/CuI nanostructure as active electrode matter for supercapacitors: A comparative investigation within two aqueous electrolytes, *Journal of Energy Storage*, 63 (2023) 107077.
8. H. Shahinfard, M. Shabani-Nooshabadi, **A. Reisi-Vanani**, R. Darabi, Electrochemical sensor based on CuO/reduced graphene nanoribbons and ionic liquid for simultaneous determination of tramadol, olanzapine and acetaminophen, *Carbon Letters*, (2023) 1-12.
9. Z. Tabandeh, **A. Reisi-Vanani**, Manipulation of the CO₂ capture capability of graphdiyne using transition metal decoration and charge injection: A DFT-D2 study, *Fuel*, 333 (2023) 126295.
10. A. Meftahi, **A. Reisi-Vanani**, M. Shabani-Nooshabadi, Comparison of performance of CuI/g-C₃N₄ nanocomposites synthesized on Ni-foam and graphitic substrates as suitable electrode materials for supercapacitors, *Fuel*, 331 (2023) 125683.
11. M. Dehkhodaei, **A. Reisi-Vanani**, The effect of the electric field intensity on the hydrogen storage of B/N-co-doped graphdiyne nanosheet, *International Journal of Hydrogen Energy*, 47 (2022) 36886-36897.
12. H. Shahinfard, M. Shabani-Nooshabadi, **A. Reisi-Vanani**, H. Ansarinejad, A novel platform based on CoMn₂O₄-rGO/1-ethyl-3-methylimidazolium chloride modified carbon paste electrode for voltammetric detection of pethidine in the presence morphine and olanzapine, *Chemosphere*, 301 (2022) 134710.
13. A. Meftahi, M. Shabani-Nooshabadi, **A. Reisi-Vanani**, AgI/g-C₃N₄ nanocomposite as electrode material for supercapacitors: Comparative study for its efficiency in three different aqueous electrolytes, *Electrochimica Acta*, 430 (2022) 141052.
14. M. Dehkhodaei, **A. Reisi-Vanani**, Effect of the charge injection and N and S co-doping on the structural and electronic properties, and hydrogen storage capacity of graphdiyne 2D structure, *Surfaces and Interfaces*, 31 (2022) 102031.
15. K. Boezar, **A. Reisi-Vanani**, M. Dehkhodaei, Modification of graphenylene nanostructure with transition metals (Fe, Sc and Ti) to promote hydrogen storage

- ability: A DFT-D3 study, *International Journal of Hydrogen Energy*, 46 (2021) 38370-38380.
16. Z. Tabandeh, **A. Reisi-Vanani**, Investigation of the adsorption behavior of two anticancer drugs on the pristine and BN-doped graphdiyne nanosheet: A DFT-D3 perception. *Diamond and Related Materials*, 119 (2021) 108564.
 17. Z. Mirzaie, **A. Reisi-Vanani**, M. Barati, S.M. Atyabi, The drug release kinetics and anticancer activity of the GO/PVA-curcumin nanostructures: The effects of the preparation method and the GO amount. *Journal of Pharmaceutical Sciences*, (2021).
 18. M.H. Darvishnejad, **A. Reisi-Vanani**, DFT-D3 calculations of the charge-modulated CO₂ capture of N/Sc-embedded graphyne: Compilation of some factors. *Journal of CO₂ Utilization*, 46 (2021) 101469.
 19. M.H. Darvishnejad, **A. Reisi-Vanani**, Synergetic effects of metals in graphyne 2D carbon structure for high promotion of CO₂ capturing, *Chemical Engineering Journal* 406 (2021) 126749.
 20. M. Ebadi, **A. Reisi-Vanani**, Methanol and carbon monoxide sensing and capturing by pristine and Ca-decorated graphdiyne: A DFT-D2 study, *Physica E: Low-dimensional Systems and Nanostructures* 125 (2021) 114425.
 21. F. Mofidi, **A. Reisi-Vanani**, Investigation of the electronic and structural properties of graphyne oxide toward CO, CO₂ and NH₃ adsorption: A DFT and MD study, *Applied Surface Science* 507 (2020) 145134.
 22. M.H. Darvishnejad, **A. Reisi-Vanani**, Density functional theory study of CO₂ capture and storage promotion using manipulation of graphyne by 3d and 4d transition metals. *International Journal of Quantum Chemistry*, 120 (2020) e26342.
 23. M.H. Darvishnejad, **A. Reisi-Vanani**, Multiple CO₂ capture in pristine and Sr-decorated graphyne: A DFT-D3 and AIMD study, *Computational Materials Science* 176 (2020) 109539.
 24. M. Algarra, J. Soto, L. Pinto da Silva, M.S. Pino-González, J.E. Rodríguez-Borges, J. Mascetti, F. Borget, **A. Reisi-Vanani**, R. Luque, Insights into the Photo-Decomposition of Azidomethyl Methyl Sulfide: A S2/S1 Conical Intersection on Nitrene Potential Energy Surfaces Leads to Formation of S-Methyl-N-Sulphenylmethanimine, *The Journal of Physical Chemistry A* 124 (2020) 1911-1921.

25. H. Teymourinia, M. Hossein Darvishnejad, O. Amiri, M. Salavati-Niasari, **A. Reisi-Vanani**, E. Ghanbari, H. Moayedi, GQDs/Sb₂S₃/TiO₂ as a co-sensitized in DSSs: Improve the power conversion efficiency of DSSs through increasing light harvesting by using as-synthesized nanocomposite and mirror, *Applied Surface Science* 512 (2020) 145638.
26. 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* 40 (2020) 693–704.
27. 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.
28. 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.
29. 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*, 50 (2019) 380-387.
30. 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.
31. 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.
32. 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.

33. 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.
34. 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.
۳۵. نرگس صائمی، مهدی شهبانی نوش آبادی، سعید معصوم، عادل رئیسی وانانی، بررسی خواص بازدارندگی شیف بیس[۲- (فنیل تیو) بنزیلیدن] ۱و۴- 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) ۷۳-۶۱.
۳۶. عادل رئیسی وانانی، فاطمه حاجیزاده، بررسی خصلت آروماتیکی برخی نانوساختارهای کربنی پلی سیکلی کاسه ای شکل، شیمی کاربردی دانشگاه سمنان، ۴۴ (۲۰۱۷) ۱۲۰-۱۰۹.
37. **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.
38. **A. Reisi-Vanani**, Z. Shabani, Evaluation of the hydrogen adsorption onto Li and Li + decorated circumtrindene (C₃₆H₁₂): A theoretical study, *International Journal of Hydrogen Energy*, 42 (2017) 22973-22986.
39. **A. Reisi-Vanani**, M. Safipoor, Investigation of carbon monoxide adsorption onto sumanene (C₂₁H₁₂) decorated with Li⁺ ions toward its elimination, *Current Applied Physics*, 17 (2017) 1382-1395.
40. **A. Reisi-Vanani**, S. Hoseinpour, A theoretical investigation of decomposition and reactivity of the atmospheric C₃F₇OCH₂O radical, *Arabian Journal of Chemistry*, 10 (2017) S1604-S1612.
41. 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.

42. **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.
43. **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.
44. **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.
45. **A. Reisi-Vanani**, S. Faghih, 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.
46. **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.
47. S. Nasiri Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Ab initio and TD-DFT study of the structural and spectroscopic properties of C₃₀H₁₀ as a new buckybowll, *Fullerenes, Nanotubes and Carbon Nanostructures*, 24 (2016) 577-587.
48. S. Hoseinpour, **A. Reisi-Vanani**, A mechanistic study for decomposition and reactivity of the C₄F₉OC₂H₄O radical derived from HFE-7200 between 200–400 K, *Progress in Reaction Kinetics and Mechanism*, (2016).
49. **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.
50. **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.
51. **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.

52. **A. Reisi-Vanani**, S. Hoseinpour, A computational study of the mechanism and kinetics for gas-phase decomposition and reactivity of the $C_4F_9OCH_2O$ radical between 200 and 400 K, *Progress in Reaction Kinetics and Mechanism*, 40 (2015) 59-68.
53. V. Jabbari, M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, D. Villagran, In,V-codoped TiO_2 nanocomposite prepared via a photochemical reduction technique as a novel high efficiency visible-light-driven nanophotocatalyst, *RSC Advances*, 5 (2015) 78128-78135.
54. 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.
55. **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.
56. **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.
57. **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.
58. **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.
59. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, V. Jabbari, Photodeposition-assisted synthesis of novel nanoparticulate In, S-codoped TiO_2 powders with high visible light-driven photocatalytic activity, *Applied Surface Science*, 285 (2013) 121-129.
60. M. Hamadani, A. Reisi-Vanani, M. Behpour, A. Esmaeily, Synthesis and characterization of Fe, S-codoped TiO_2 nanoparticles: Application in degradation of organic water pollutants, *Desalination*, 281 (2011) 319-324.

61. 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.
62. 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.
63. 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. A. Masiha, **A. Reisi-Vanani**, Examining the hydrogenation of CO₂ utilizing a single metal catalyst of Mn embedded into g-C₃N₄ (heptazine), 22nd Iranian Chemistry Congress (ICC22), Iranian Research Organization for Science and Technology (IROST) 13-15 May, 2024.
2. A. Masiha, **A. Reisi-Vanani**, Investigation of the CO₂ reduction reaction employing Cr single metal catalyst embedded onto g-C₃N₄ (heptazine), 22nd Iranian Chemistry Congress (ICC22), Iranian Research Organization for Science and Technology (IROST) 13-15 May, 2024.
3. G. Jafari, **A. Reisi-Vanani**, Transition metals embedded 8-16-4 graphyne: Investigation of the structural, electronic and magnetic properties, 22nd Iranian Chemistry Congress (ICC22), Iranian Research Organization for Science and Technology (IROST) 13-15 May, 2024.
4. Sima Roshan, **A. Reisi-Vanani**, M.R. Delavarian, Computational study of the carbon dioxide hydrogenation to formic acid on to Ni,N/graphyne, 4th Iranian Catalyst Conference, Iran University of Science & Technology, 28-29 Jan, 2024.
5. Sima Roshan, **A. Reisi-Vanani**, M.R. Delavarian, Nitrogen-doped graphyne nanosheet for CO₂ reduction reaction: A DFT calculation, 4th Iranian Catalyst Conference, Iran University of Science & Technology, 28-29 Jan, 2024.
6. Sima Roshan, **A. Reisi-Vanani**, Simin Roshan, The Effect of Vanadium Atom Metal Decorations to Promote Hydrogen Adsorption Capacity of Borophene Structure: A

- DFT Study, 9th International Congress on Nanoscience & Nanotechnology, ICNN2022, University of Tehran, Tehran, March 1-2, **2023**.
7. Simin Roshan, **A. Reisi-Vanani**, Sima Roshan, Manipulation of Hydrogen Adsorption Capability on Borophene Nanosheet Using Chromium Atom Metal Decorations, 9th International Congress on Nanoscience & Nanotechnology, ICNN2022, University of Tehran, Tehran, March 1-2, **2023**.
 8. Z. Tabandeh, **A. Reisi-Vanani**, CO₂ capturing by Cr-graphdiyne surface: A DFT-D2 computational study, 21st Iranian Chemistry Congress, Azarbayegan Shahid Madani University, 26-28 Jul **2022**.
 9. Simin Roshan, **A. Reisi-Vanani**, Sima Roshan, Modification of the structural and electronic properties of Ni decorated borophene for hydrogen adsorption: A DFT study, 23rd Iranian Physical Chemistry Conference, Shahid Bahonar University of Kerman, 12-13 Jan **2022**.
 10. Sima Roshan, **A. Reisi-Vanani**, Simin Roshan, DFT study of promote hydrogen adsorption by borophene nanostructure decorated with Sc atom, 23rd Iranian Physical Chemistry Conference, Shahid Bahonar University of Kerman, 12-13 Jan **2022**.
 11. M. Dehkhodaei, **A. Reisi-Vanani**, Computational study of the synergistic effect of N,S atoms co-doping into monolayer graphdiyne nanosheet on hydrogen adsorption and storage, 23rd Iranian Physical Chemistry Conference, Shahid Bahonar University of Kerman, 12-13 Jan **2022**.
 12. Simin Roshan, **A. Reisi-Vanani**, Influence of Titanium and Zinc atoms decoration on the electronical and structural properties of β 12-borophene, 8th International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, **2021**.
 13. Sima Roshan, **A. Reisi-Vanani**, Simin Roshan, Evaluation of the vanadium-decorated borophene nano-sheet as a hydrogen storage medium, 8th International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, **2021**.
 14. Sima Roshan, **A. Reisi-Vanani**, Modification of the electronic and structural properties of β 12 borophene nanosheet by scandium and copper atoms decoration, 8th

- International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, **2021**.
15. Z. Mirzaie, M. Barati, **A. Reisi-Vanani**, Synthesis of Poly (vinyl alcohol)-Sodium Alginate/Graphene Oxide films for controlled release of the anticancer drug curcumin, 11st International Chemical Engineering congress & Exhibition (IChEC 2020) Fouman (Pardis of Tehran University), Iran, 28-30 Oct, **2020**.
 16. Z. Tabandeh, **A. Reisi-Vanani**, A First Principles Study of the Interaction of Graphdiyne Nanosheet with Hydroxyurea Anticancer Drug, 8th International Conference on Nanostructures (ICNS8), Sharif University of Technology, 18-20 Nov **2020**.
 17. F. Mofidi-Bidgoli, **A. Reisi-Vanani**, Titanium Decorated Graphyne As Sensor of Sarin: A DFT-D study, 9th National Seminar of Chemistry and Environment, Arak University, 3-4 Sep **2019**.
 18. F. Mofidi-Bidgoli, **A. Reisi-Vanani**, Sensing Ammonia (NH₃) By Graphyne and Graphyne Oxide, 9th National Seminar of Chemistry and Environment, Arak University, 3-4 Sep **2019**.
 19. K. Boezar, **A. Reisi-Vanani**, DFT-D study of hydrogen storage onto Fe decorated monolayer graphenylene, 21st Iranian Inorganic Chemistry Conference, Arak University, 28-29 Aug **2019**.
 20. K. Boezar, **A. Reisi-Vanani**, Evaluation of electronic and structural properties of scandium decorated graphenylene: A DFT-D3 study, 21st Iranian Inorganic Chemistry Conference, Arak University, 28-29 Aug **2019**.
 21. M. Akbari, **A. Reisi-Vanani**, S. Shamae, Modification of graphdiyne by vanadium single atom to promote hydrogen adsorption, 22nd Iranian Physical Chemistry Conference, Zanzan University, 20-22 Aug **2019**.
 22. M. Akbari, **A. Reisi-Vanani**, Electronic and structural properties of Sc decorated graphdiyne toward hydrogen adsorption, 22nd Iranian Physical Chemistry Conference, Zanzan University, 20-22 Aug **2019**.
 23. S. Shamae, **A. Reisi-Vanani**, Titanium decorated graphdiyne as a hydrogen storage medium, 22nd Iranian Physical Chemistry Conference, Zanzan University, 20-22 Aug **2019**.

۲۴. عادل رئیسی وانانی، زهرا میرزایی، محمد براتی، کامپوزیت پلی وینیل الکل-سدیم آلزینات-گرافن اکساید به عنوان

یک سیستم رهاسازی کنترل شده برای داروی کورکومین، چهارمین کنفرانس شیمی کاربردی ایران، دانشگاه ارومیه،

۱-۳ مرداد ۱۳۹۸.

25. M. H. Darvishnejad, **A. Reisi-Vanani**, F. Akbari, Effect of the Al doping on the electronic and structural properties of γ -graphyne: A DFT study, ICNN 2018, Research Institute Petroleum Industry, Tehran, 26-28 Sep **2018**.
26. M. H. Darvishnejad, **A. Reisi-Vanani**, Adsorption Properties of the Phosgene Gas on Bilayer γ -Graphyne: A DFT study, ICNN 2018, Research Institute Petroleum Industry, Tehran, 26-28 Sep **2018**.
27. F. Mofidi-Bidgoli, **A. Reisi-Vanani**, DFT study of the carbon monoxide adsorption onto graphyne oxide, ICNN 2018, Research Institute Petroleum Industry, Tehran, 26-28 Sep **2018**.
28. M. Asgari-Bajgirani, **A. Reisi-Vanani**, DFT study of the structural properties of various stacked bilayer graphdiyne and HCN adsorption, 21st Iranian Physical Chemistry Conference, Azarbaijan Shahid Madani University, 6-8 Sep **2018**.
29. M. Ebadi, **A. Reisi-Vanani**, F. Houshmand, Electronic, Magnetic and Structural Properties of Calcium Decorated Carbon 2D Structure (Graphdiyne), 7th International Conference on Nanostructures (ICNS7), Sharif University of Technology, 27 Feb-1 Mar **2018**.
30. 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**.
31. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, The structure and spectroscopic properties of $C_{30}H_{10}$ 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**.
32. 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**.

33. **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**.
34. **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**.
35. **A. Reisi-Vanani**, Z. Shabani, Effect of Li and Li⁺ decorating in circumtrindene (C₃₆H₁₂) frame toward hydrogen adsorption: A theoretical study, 19th Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
36. **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**.
37. **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**.
38. 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**.
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