

## IN THE NAME OF GOD

### Curriculum Vitae

*Dr. Adel Reisi-Vanani*

Associate Professor of Physical Chemistry

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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 (M.Sc.)

### **Journal Publications:**

1. 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.
2. 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).
3. M.H. Darvishnejad, **A. Reisi-Vanani**, DFT-D3 calculations of the charge-modulated CO<sub>2</sub> capture of N/Sc-embedded graphyne: Compilation of some factors. *Journal of CO<sub>2</sub> Utilization*, 46 (2021) 101469.
4. M.H. Darvishnejad, **A. Reisi-Vanani**, Synergetic effects of metals in graphyne 2D carbon structure for high promotion of CO<sub>2</sub> capturing, *Chemical Engineering Journal* 406 (2021) 126749.
5. 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.
6. F. Mofidi, **A. Reisi-Vanani**, Investigation of the electronic and structural properties of graphyne oxide toward CO, CO<sub>2</sub> and NH<sub>3</sub> adsorption: A DFT and MD study, *Applied Surface Science* 507 (2020) 145134.

7. M.H. Darvishnejad, **A. Reisi-Vanani**, Density functional theory study of CO<sub>2</sub> capture and storage promotion using manipulation of graphyne by 3d and 4d transition metals. *International Journal of Quantum Chemistry*, 120 (2020) e26342.
8. M.H. Darvishnejad, **A. Reisi-Vanani**, Multiple CO<sub>2</sub> capture in pristine and Sr-decorated graphyne: A DFT-D3 and AIMD study, *Computational Materials Science* 176 (2020) 109539.
9. 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 S<sub>2</sub>/S<sub>1</sub> Conical Intersection on Nitrene Potential Energy Surfaces Leads to Formation of S-Methyl-N-Sulfenylmethanimine, *The Journal of Physical Chemistry A* 124 (2020) 1911-1921.
10. H. Teymourinia, M. Hossein Darvishnejad, O. Amiri, M. Salavati-Niasari, **A. Reisi-Vanani**, E. Ghanbari, H. Moayedi, GQDs/Sb<sub>2</sub>S<sub>3</sub>/TiO<sub>2</sub> 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.
11. S.K. Nasiri, **A. Reisi-Vanani**, M. Hamadani, Molecular Structure, Spectroscopic, Local and Global Reactivity Descriptors and NBO Analysis of C<sub>32</sub>H<sub>12</sub>: A New Buckybowl and Sub-Fullerene Structure, *Polycyclic Aromatic Compounds* 40 (2020) 693–704.
12. 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.
13. F. Mofidi, **A. Reisi-Vanani**, Sensing and elimination of the hazardous materials such as Sarin by metal functionalized  $\gamma$ -graphyne surface: A DFT study, *Journal of Molecular Liquids*, 286 (2019) 110929.
14. 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).

15. M. Shams, **A. Reisi-Vanani**, Potassium decorated  $\gamma$ -graphyne as hydrogen storage medium: Structural and electronic properties, *International Journal of Hydrogen Energy*, 44 (2019) 4907-4918.
16. 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.
17. 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( $\epsilon$ -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.
18. 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.
19. 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.
۲۰. نرگس صائمی، مهدی شبانی نوش آبادی، سعید معصوم، عادل رئیسی وانانی، بررسی خواص بازدارندگی شیف بیس [۲- (فنیل تیو) بنزیلیدن] او۴-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.
۲۱. عادل رئیسی وانانی، فاطمه حاجیزاده، بررسی خصلت آروماتیکی برخی نانوساختارهای کربنی پلی سیکلی کاسه ای شکل، شیمی کاربردی دانشگاه سمنان، ۴۴ (۲۰۱۷) ۱۲۰-۱۰۹.
22. **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.

23. **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.
24. **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.
25. 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.
26. 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.
27. **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.
28. **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.
29. **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.
30. **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.
31. **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.

32. S. Nasiri Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Ab initio and TD-DFT study of the structural and spectroscopic properties of C<sub>30</sub>H<sub>10</sub> as a new bucky bowl, *Fullerenes, Nanotubes and Carbon Nanostructures*, 24 (2016) 577-587.
33. S. Hoseinpour, **A. Reisi-Vanani**, A mechanistic study for decomposition and reactivity of the C<sub>4</sub>F<sub>9</sub>OC<sub>2</sub>H<sub>4</sub>O radical derived from HFE-7200 between 200–400 K, *Progress in Reaction Kinetics and Mechanism*, (2016).
34. **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.
35. **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.
36. **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.
37. **A. Reisi-Vanani**, S. Hoseinpour, A computational study of the mechanism and kinetics for gas-phase decomposition and reactivity of the C<sub>4</sub>F<sub>9</sub>OCH<sub>2</sub>O radical between 200 and 400 K, *Progress in Reaction Kinetics and Mechanism*, 40 (2015) 59-68.
38. V. Jabbari, M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, D. Villagran, In,V-codoped TiO<sub>2</sub> nanocomposite prepared via a photochemical reduction technique as a novel high efficiency visible-light-driven nanophotocatalyst, *RSC Advances*, 5 (2015) 78128-78135.
39. 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.
40. **A. Reisi-Vanani**, S. Faghih, 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.
41. **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.

42. **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.
43. **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.
44. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, V. Jabbari, Photodeposition-assisted synthesis of novel nanoparticulate In, S-codoped TiO<sub>2</sub> powders with high visible light-driven photocatalytic activity, *Applied Surface Science*, 285 (2013) 121-129.
45. M. Hamadani, **A. Reisi-Vanani**, M. Behpour, A. Esmaily, Synthesis and characterization of Fe, S-codoped TiO<sub>2</sub> nanoparticles: Application in degradation of organic water pollutants, *Desalination*, 281 (2011) 319-324.
46. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Sol-gel preparation and characterization of Co/TiO<sub>2</sub> nanoparticles: application to the degradation of methyl orange, *Journal of the Iranian Chemical Society*, 7 (2010) S52-S58.
47. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Synthesis, characterization and effect of calcination temperature on phase transformation and photocatalytic activity of Cu, S-codoped TiO<sub>2</sub> nanoparticles, *Applied Surface Science*, 256 (2010) 1837-1844.
48. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Preparation and characterization of S-doped TiO<sub>2</sub> nanoparticles, effect of calcination temperature and evaluation of photocatalytic activity, *Materials Chemistry and Physics*, 116 (2009) 376-382.

#### Conference papers:

1. Simin Roshan, **A. Reisi-Vanani**, Influence of Titanium and Zinc atoms decoration on the electronical and structural properties of  $\beta$ 12-borophene, 8<sup>th</sup> International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, 2021.

2. Sima Roshan, **A. Reisi-Vanani**, Simin Roshan, Evaluation of the vanadium-decorated borophene nano-sheet as a hydrogen storage medium, 8<sup>th</sup> International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, **2021**.
3. Sima Roshan, **A. Reisi-Vanani**, Modification of the electronic and structural properties of  $\beta$ 12 borophene nanosheet by scandium and copper atoms decoration, 8<sup>th</sup> International E-congress on Nanosciences and Nanotechnology (ICNN 2021), Mashhad University of Medical Sciences, 17-18 Feb, **2021**.
4. 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, 11<sup>th</sup> International Chemical Engineering congress & Exhibition (IChEC 2020) Fouman (Pardis of Tehran University), Iran, 28-30 Oct, **2020**.
5. Z. Tabandeh, **A. Reisi-Vanani**, A First Principles Study of the Interaction of Graphdiyne Nanosheet with Hydroxyurea Anticancer Drug, 8<sup>th</sup> International Conference on Nanostructures (ICNS8), Sharif University of Technology, 18-20 Nov **2020**.
6. F. Mofidi-Bidgoli, **A. Reisi-Vanani**, Titanium Decorated Graphyne As Sensor of Sarin: A DFT-D study, 9<sup>th</sup> National Seminar of Chemistry and Environment, Arak University, 3-4 Sep **2019**.
7. F. Mofidi-Bidgoli, **A. Reisi-Vanani**, Sensing Ammonia (NH<sub>3</sub>) By Graphyne and Graphyne Oxide, 9<sup>th</sup> National Seminar of Chemistry and Environment, Arak University, 3-4 Sep **2019**.
8. K. Boezar, **A. Reisi-Vanani**, DFT-D study of hydrogen storage onto Fe decorated monolayer graphenylene, 21<sup>th</sup> Iranian Inorganic Chemistry Conference, Arak University, 28-29 Aug **2019**.
9. K. Boezar, **A. Reisi-Vanani**, Evaluation of electronic and structural properties of scandium decorated graphenylene: A DFT-D3 study, 21<sup>th</sup> Iranian Inorganic Chemistry Conference, Arak University, 28-29 Aug **2019**.
10. M. Akbari, **A. Reisi-Vanani**, S. Shamae, Modification of graphdiyne by vanadium single atom to promote hydrogen adsorption, 22<sup>th</sup> Iranian Physical Chemistry Conference, Zanjan University, 20-22 Aug **2019**.



11. M. Akbari, **A. Reisi-Vanani**, Electronic and structural properties of Sc decorated graphdiyne toward hydrogen adsorption, 22<sup>th</sup> Iranian Physical Chemistry Conference, Zanjan University, 20-22 Aug **2019**.
  12. S. Shamae, **A. Reisi-Vanani**, Titanium decorated graphdiyne as a hydrogen storage medium, 22<sup>th</sup> Iranian Physical Chemistry Conference, Zanjan University, 20-22 Aug **2019**.
۱۳. 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.
14. M. H. Darvishnejad, **A. Reisi-Vanani**, F. Akbari, Effect of the Al doping on the electronic and structural properties of  $\gamma$ -graphyne: A DFT study, ICNN 2018, Research Institute Petroleum Industry, Tehran, 26-28 Sep **2018**.
  15. M. H. Darvishnejad, **A. Reisi-Vanani**, Adsorption Properties of the Phosgene Gas on Bilayer  $\gamma$ -Graphyne: A DFT study, ICNN 2018, Research Institute Petroleum Industry, Tehran, 26-28 Sep **2018**.
  16. 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**.
  17. M. Asgari-Bajgirani, **A. Reisi-Vanani**, DFT study of the structural properties of various stacked bilayer graphdiyne and HCN adsorption, 21<sup>th</sup> Iranian Physical Chemistry Conference, Azarbaijan Shahid Madani University, 6-8 Sep **2018**.
  18. M. Ebadi, **A. Reisi-Vanani**, F. Houshmand, Electronic, Magnetic and Structural Properties of Calcium Decorated Carbon 2-D Structure (Graphdiyne), 7<sup>th</sup> International Conference on Nanostructures (ICNS7), Sharif University of Technology, 27 Feb-1 Mar **2018**.
  19. M. Shams-Ghamsari, **A. Reisi-Vanani**, DFT study of potassium decorated  $\gamma$ -graphyne: Electronic structure and optical properties, 20<sup>th</sup> Iranian Physical Chemistry Conference, University of Arak, 20-22 Aug **2017**.
  20. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadian, The structure and spectroscopic properties of C<sub>30</sub>H<sub>10</sub> as a new bucky bowl: DFT and TD-DFT study, 2<sup>nd</sup> international

conference on new research achievement in chemistry and chemical engineering, 5 May **2016**.

21. 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, 2<sup>nd</sup> international conference on new research achievement in chemistry and chemical engineering, 5 May **2016**.
22. **A. Reisi-Vanani**, F. Hajizadeh, Theoretical study of dithiaporphyrin as sensitizer for dye-sensitized solar cells application, 19<sup>th</sup> Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
23. **A. Reisi-Vanani**, M. Safipour, Computational investigation of the adsorption of CO on the Li<sup>+</sup>-decorated sumanene, 19<sup>th</sup> Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
24. **A. Reisi-Vanani**, Z. Shabani, Effect of Li and Li<sup>+</sup> decorating in circumtrindene ( $C_{36}H_{12}$ ) frame toward hydrogen adsorption: A theoretical study, 19<sup>th</sup> Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
25. **A. Reisi-Vanani**, S. Bahramian, Theoretical study of the sumanene nanostructure functionalization by diazomethane in the gas phase using density functional theory, 19<sup>th</sup> Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
26. **A. Reisi-Vanani**, S.N. Kokhdan, M. Hamadani, Computational study of the gas phase reaction of HNCO and sumanene: A DFT study, 19<sup>th</sup> Iranian Physical Chemistry Conference, University of Guilan, 13-15 September **2016**.
27. 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, 18<sup>th</sup> Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
28. **A. Reisi-Vanani**, S. Mehrdoust, Theoretical Study of the Hydrogen Adsorption on Sumanene Nanostructure and its Boron Doped Derivatives: A Density Functional Theory Study, 18<sup>th</sup> Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.

29. S.N. Kokhdan, **A. Reisi-Vanani**, M. Hamadani, Theoretical study on the mechanism of cycloaddition reaction of nitrous oxide onto sumanene nanostructure, 18<sup>th</sup> Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
30. **A. Reisi-Vanani**, F. Shamsali, Quantum Study of the Hydrogen Adsorption on Nitrogen-doped Sumanene Nanostructure: A DFT and MP2 Study, 18<sup>th</sup> Iranian Chemistry Congress, University of Semnan, 30 August-1 September **2015**.
۳۱. 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- فنیل دی آمین با استفاده از طراحی آزمایش آماری، شانزدهمین کنگره ملی خوردگی، پژوهشگاه صنعت نفت، ۳ و ۴ آذر ۱۳۹۴.
32. S. Rahimi, **A. Reisi-Vanani**, Theoretical study of the 1,3- dipolar cycloaddition of hydrogen azide to corannulene nanostructure ,17<sup>th</sup> Iranian Physical Chemistry Conference, University of Khaje-nasire-toosi, 21-23 October **2014**.
33. S. Faghih, **A. Reisi-Vanani**, Computational study of hydrogen storage on corannulene and its hydroxyl derivatives, 20<sup>th</sup> Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
34. L. Alihoseini, **A. Reisi-Vanani**, Theoretical investigation of hydrogen storage in corannulene and its nitrogen derivatives, 20<sup>th</sup> Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
35. L. Shahrokh, **A. Reisi-Vanani**, Theoretical study of the kinetics of the reaction of hydroxyl radical with corannulene nanostructure, 20<sup>th</sup> Iranian Seminar of Organic Chemistry, Bu-Ali Hamedan, 3-5 July **2013**.
36. S. Hoseinpour, **A. Reisi-Vanani**, Maryam Shamsiri, Rationalization of two-step mechanism of functionalization of single-walled carbon nanotubes with aryl diazonium salts: Comparison of OH and CH<sub>2</sub>CH<sub>3</sub> substituent groups, Seminar of calculation in nanotechnology, Azad University, Oloum darouee branch, 16 February **2013**.
37. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, Combining Sol-Gel and Hydrothermal Methods With Photodeposition Method to Prepare In/TiO<sub>2</sub>

- Nanoparticles, Iran-Belarus International Conference on Modern Applications of Nanotechnology (IBCN12), Minsk, Belarus, June 27-29, **2012**.
38. **A. Reisi-Vanani**, S. Hoseinpour, Theoretical studies of decomposition and reactivity of the  $C_3F_7OCH_2O$ , 15<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, September 4-6, **2012**.
  39. **A. Reisi-Vanani**, S. Hoseinpour, Ab initio studies on the reactivity and thermal decomposition of the  $CF_3OCH_2O$  radical, 15<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 4-6, **2012**.
  40. M. Hamadani, **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**.
  41. **A. Reisi-Vanani**, M. Hamadani, Enhancement of the photocatalytic activity of doped and co-doped  $TiO_2$  nanoparticles by metal and non-metal atoms and phase transformation, 14<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, **2011**.
  42. Z. Tavangar, M. Hamadani, **A. Reisi-vanani**, Effect of calcination temperature on Preparation, Characterization and evaluation of photocatalytic activity of Sulfur doped  $TiO_2$  nanoparticles, 11<sup>th</sup> Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
  43. M. Hamadani, **A. Reisi-vanani**, Synthesis, characterization and effect of calcinations temperature on phase transformation and photocatalytic activity of Cu,S-codoped  $TiO_2$  nanoparticles, 11<sup>th</sup> Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
  44. **A. Reisi-Vanani**, M. Hamadani, Sol-gel preparation of Cu,S-codoped  $TiO_2$  nanoparticles and evaluation of phase transformation and photocatalytic activity, 13<sup>th</sup> Iranian Seminar of Physical Chemistry, Shiraz University, April **2010**.
  45. **A. Reisi-Vanani**, M. Hamadani, 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**.

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