Zahra Tavangar
Department of Physical Chemistry
Faculty of Chemistry
University of Kashan, I. R. Iran.
Km 6 Qotb-e Ravandi Blvd,
Kashan, Iran, 8731753153.

Email: z.tavangar@kashanu.ac.ir Homepage: faculty.kashanu.ac.ir

Education

2009 **Ph.D.** Physical Chemistry, Isfahan University, Isfahan, Iran
Dissertation title: Molecular Dynamic Simulation of Fluid Flow through Carbon Nanotube Junctions

1997 ***M.Sc.*** Physical Chemistry, Buali Sina University, Hamedan, Iran
Thesis title: Direct Determination of the Intermolecular Potential of Kr-N_2, Xe-N_2 and He-SF_6 from the Extended Principle of Corresponding States

1994 ***B.Sc.*** Pure Chemistry, Isfahan, Iran

Employment

2009- University of Kashan, Faculty of chemistry, Department of Physical chemistry, Associate professor of Physical Chemistry

2005-2009 Isfahan university, Faculty of science, Department of Chemistry, Teacher Assistant

1999-2003 University of Kashan, Faculty of chemistry, Department of Physical Chemistry, Teacher Assistant

Research Interest

1. **Quantum chemistry**
   - Molecular modeling
   - Density functional theory
   - Quantum mechanical ab initio methods
   - Semi-empirical methods.
   - Car-Parrinello molecular dynamics
2. **Molecular dynamical simulation**

Management Experience

2014-2018: Head of Physical Chemistry, University of Kashan, Kashan, Iran.
2022-Present: Head of Physical Chemistry, University of Kashan, Kashan, Iran.

Honors

2015: Distinguished Teacher, Faculty of Chemistry, University of Kashan
2018: Distinguished Teacher, Faculty of Chemistry, University of Kashan
2022: Distinguished Teacher, Faculty of Chemistry, University of Kashan

2023: Distinguished researcher, Faculty of Chemistry, University of Kashan
2025: Distinguished Teacher, Faculty of Chemistry, University of Kashan

Teaching Experience

Advanced Physical Chemistry
Quantum Chemistry
Statistical Thermodynamic
Advanced Chemical Kinetics
Computational Chemistry
Molecular Spectroscopy
Computer in Chemistry
General Chemistry
Laboratory of Physical Chemistry

Publications:

A) Journal Papers

1- M. R. Zamani Seyfikar, Z. Tavangar, "Tunable sensing, capture, and dissociation of CO and CO_2 on doped, 3d-transition-metal-decorated h-BN: A DFT study", *Materials Chemistry and Physics,* 359 (2026) 132529.

2- A. Ghahremani, Z. Tavangar, M. R. Zamani Seyfikar, "Computational investigation of mechanical properties and adsorption behavior of sulfur-doped h-BN nanosheets", *Scientific Reports,* 15 (2025) 32113.

3- H. Pirdadeh Beyranvand, Z. Tavangar, "Electrochemical reduction of CO_2 on S-triazine-based g-C_3N_4 surface modified with metal and nonmetal atoms: A DFT study", *Journal of CO_2 Utilization,* 97 (2025) 103123.

4- M. Mohammadi, Z. Tavangar, "Effect of strain and charge injection on pollutant molecule sensing using black phosphorene: A DFT study", *Applied Surface Science,* 698 (2025) 163114.

5- H. Basreh Arani, Z. Tavangar, F. Zergani, "High sensitivity of s-triazine based g-C_3N_4 surface to pollutant gases", *Applied Surface Science,* 659 (2024) 159926.

6- M. Afzalkhah, S. Masoum, M. Behpour, Z. Tavangar, H. Naeimi, "Corrosion inhibition behavior of 2-(4-methoxyphenyl)-benzothiazole on mild steel corrosion through design of experiments approach, quantum chemical calculations and molecular dynamics simulation", *Journal of the Iranian Chemical Society*, 21 (2024) 211439.

7- F. Zergani, Z. Tavangar, "Achieving arbitrary CO_2 adsorption energy on χ3 borophene surface by applying electric field or strain: DFT and RSM approaches", *Fuel,* 350 (2023) 128809.

8- M. Heshami, Z. Tavangar, B. Taheri, "Adsorption of gold and silver glycinate on graphene and graphene oxide surface: A DFT study", *Applied Surface Science,* 619 (2023) 156676.

9- M. Mohammadi, Z. Tavangar, "Adsorption of aromatic molecules on a black phosphorene surface: a first-principles study", *New Journal of Chemistry,* 47 (2023) 1842.

10- M. Mazloum-Ardakani, A. Ebadi, Z. Tavangar, F. Vajhadin, R. Behjatmanesh-Ardakani, S. M. Moshtaghioun, R. Haghniaz, "Fabrication of pH-Sensitive Dual Antibiotic-Loaded PVP-PEG@ZnO Nanohybrids for Controlled Drug Release to Combat Bacteria", *Journal of Nanostructures,* 12 (2022) 389.

11- F. Vajhadin, M. Mazloum-Ardakani, Z. Tavangar, M. Shahidi, "Design of a nanocytosensor for isolation and electrochemical detection of folate-overexpressed circulating tumor cells", *Sensors and Actuators: B. Chemical,* 365 (2022) 131873.

12- F. Zergani, Z. Tavangar, "Gas sensing behavior and adsorption mechanism on χ3 borophene surface", *Chemical Engineering Journal,* 431 (2022) 133947.

13- Z. Hajiahmadi, Z. Tavangar, "Proposing a new complexing agent for cyanide-free silver electroplating through a comprehensive computational study of dimethyl hydantoin", *Molecular Simulation,* 47 (2021) 619–627.

14- H. Pirdadeh Beyranvand, Z. Tavangar, "A detailed study of lithium storage on γ-BNyne; computational approach", *Applied Surface Science,* 542 (2021) 148569.

15- Z. Hajiahmadi, Z. Tavangar, H. Behzadi "A DFT Study of the reaction between benzopyrene epoxide and C_{60} derivatives as possible anticancer activity", *Polycyclic Aromatic Compounds,* 41 (2021) 593.

16- F. Zergani, Z. Tavangar, "A thorough study on the F-decoration of χ3 borophene and enhancement of anodic performance of Lithium-ion batteries", *Journal of Molecular Liquids,* 319 (2020) 114343.

17- P. Mehdizadeh, Z. Tavangar, N. Shabani, M. Hamadanian "Visible light activity of nitrogen-doped TiO2 by Sol-Gel method using various nitrogen sources", *Journal of Nanostructures,* 10, (2020) 307.

18- S. Tahmasebi, Z. Tavangar, M. Hamadanian, "Using of Artemesia Absinthinum, Verbascum Thapsus, Viola Odorata, Matricaria Chamomilla and Corianderum Satirum Natural Dyes in Making Dyesensitized Solar Cells", *Advanced Materials Materials and Novel Coatings,* 32, (2020) 2346

19- S. L. Fani, Z. Tavangar, A. Kazempour "Boron decorated graphene nanosheet as an ultrasensitive sensor: the role of coverage", *Journal of Molecular Modeling,* 25 (2019) 166.

20- Z. Hajiahmadi, Z. Tavangar, "Extensive theoretical study of corrosion inhibition efficiency of some pyrimidine derivatives on iron and the proposal of new inhibitor", *Journal of Molecular Liquids,* 284 (2019) 225.

21- Z. Amaniseyed, Z. Tavangar, "Hydrogen storage on uncharged and positively charged Mg-decorated graphene", *International Journal of Hydrogen Energy,* 44 (2019)3803.

22- Z. Hajiahmadi, Z. Tavangar, "Investigating the adsorption of nitrobenzene on M/Pd (1 1 1) bimetallic surface as an effective catalyst", *Applied Surface Science,* 454 (2018) 343.

23- A. Payvand, Z. Tavangar, "Computational study on the functionalization of BNNC with pyrrole molecule", *Superlattices and Microstructures,* 117, (2018) 373.

24- P. Mehdizadeh, Z. Tavangar, "Photocatalyst Ag@N/TiO_2 Nanoparticles: Fabrication, Characterization, and Investigation of the Effect of Coating on Methyl Orange Dye Degradation", *Journal of Nanostructures,* 7, (2017) 216.

25- Z. Tavangar, M. Hamadanian, , H. Basharnavaz, "Studying the effects of the configuration of doped Al atoms on theconductive properties of boron nitride nanotube using density functional theory", *Chemical Physics Letters,* 669, (2017) 29.

26- M. Malehmir, B. Khoshnevisan, Z. Tavangar, “Chirality effect on Lithiation of narrow carbon nanotubes; bond order MD and DFT studies”, *Materials. Research. Express,* 3, (2016) 105015.

27- M. Hamadanian, Z. Tavangar, S. Naseh ,“The modification of benzene adsorption on zigzag single-wall carbon nanotubes by carboxylation”, *Materials. Research. Express,* 3, (2016) 125010.

28- Z. Tavangar, M. Hamadanian, , H. Basharnavaz,“ Variation of the electronic properties of zigzag boron nitride nanotubes by Al-doping: a DFT study”, *Molecular Physics,* 114, (2016) 2936.

29- Z. Tavangar, N. Zareie ,“Efficiency improvement of new Tetrathionate-based dyes by enhancing donor, acceptor and bridge units, a theoretical study”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 167 (2016) 72.

30- M. Hamadanian, Z. Tavangar, S. Naseh, “Improvement of electronic properties of carboxylated zigzag single wall carbon nanotubes by interaction with benzene derivatives”, *Current Applied Physics*, 15 (2015) 1593

31- M. Hamadanian, Z. Tavangar, B. Noori ,“Modification of conductive properties of (10, 0) zigzag single-walled carbon nanotubes (SWCNT) by alkali metals absorption”, *Journal of Molecular Structure*, 1078 (2014) 49.

32- M. Hamadanian, Z. Tavangar, B. Noori, “Modification of the electronic properties of zigzag (n=5-10) and armchair (n=3,5) carbon nanotubes by K atom adsorption”, *Structural Chemistry*, 25, 25 (2014) 1005

33- M. Hamadanian, Z. Tavangar, S. Naseh, “The structural and electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes modified by thiophene groups”, *Chemical Physics Letters*, 584 (2013) 177.

34- M. Hamadanian, B. Khoshnevisanc, F. Kalantari Fotoohd, Z. Tavangar, "Computational study of super cell Al-substituted single-walled carbon nanotubes as CO sensor", *Computational Materials Science*, 58 (2012) 45.

35- Z. Tavangar, " Diels–Alder [4+2] Cycloadditions of C20 with Some Diene and 1,2-Dioxo Compounds: A Theoretical Study", *Journal of Nanostructure*, 1 (2012) 159.

36- A. R. Ashrafi, M. Hamadanian, Z. Tavangar, H. Sabzyan, “Symmetry of a capped nanotube”, *Digest Journal of Nanomaterials and Biostructures,* 4 (2009), 319.

37- H. Sabzyan, Z. Tavangar, “Characterization of the flow of the CO/CO_2 gases through carbon nanotube junctions using molecular dynamic simulations”, *Chemical Physics,* 362 (2009), 120.

38- H. Iloukhani, Z. Tavangar, E. K. Goharshadi, “Direct determination of the intermolecular potential of Kr - N_2, Xe - N_2 and He - SF_6 from the extended principle of corresponding states”, *Indian Journal of Chemistry A,* 40 (2001), 185.

39- E. K. Goharshadi,Z. Mirafzali, Z. Tavangar, “Direct Determination of the Interaction Potentials of Sulphur Hexafluride-Noble Gases from the Extended Principle of Corresponding States”, *Journal of the Physical Society of Japan, 67* (1998), 4296.

B) Conference Papers

1- M. Esfahani, Z. Tavangar, “Computational investigation of the interaction of CO_2 and CO gas with the $\chi 6$ borophene surface”, Proceeding of 13th International Chemical Engineering Congress & Exhibition, Iranian Association of Chemical Engineering, Tehran, 10 September 2026.

2- - M. Esfahani, Z. Tavangar, “Computational study of sensing behavior and adsorption of H_2S gas on the surface of bis(Iminothiolitho)Rhodium”, Proceeding of 13th International Chemical Engineering Congress & Exhibition, Iranian Association of Chemical Engineering, Tehran, 10 September 2026.

3- M. R. Zamani Seyfikar, Z. Tavangar, “NO_2 detection and elimination using S-doped h-BN surface”, Proceeding of 23nd Iranian Inorganic Chemistry Conference, University of Qom, Qom, 6 November 2024.

۴- محمدرضا زمانی سیفی‌کار ، زهرا توانگر، "تشخیص و حذف گاز NO با استفاده از سطح h-BN دوپ شده با گوگرد"، کتابچه بیست و چهارمین کنفرانس شیمی‌فیزیک ایران، دانشگاه اصفهان، اصفهان، ۲۹ آبان‌ماه ۱۴۰۳.

۵- منصوره اصفهانی، زهرا توانگر، "بررسی محاسباتی برهمکنش گاز SO_2 با سطح بیس (ایمینوتیولیتو)رودیم"، کتابچه بیست و چهارمین کنفرانس شیمی‌فیزیک ایران، دانشگاه اصفهان، اصفهان، ۲۹ آبان‌ماه ۱۴۰۳.

6- M. R. Zamani Seyfikar, Z. Tavangar, “Computational investigation of lithium adsorption on C3N5 monolayer”, Proceeding of 1st and 2nd National Lithium Battery Conference (LBC2024), Iran University of Science and Technology, Tehran, 9 July 2024.

7- H. Pirdadeh Beyranvand, Z. Tavangar, “Structural and electronic properties of C-decorated γ-BNyne”, Proceeding of 8th International Conference on Nanostructures (ICNS8), Sharif University of Technology, Tehran, 18 November 2020.

8- F. Zergani, Z. Tavangar, “Structural and electronic properties of Si-decorated borophene χ3”, Proceeding of 8th International Conference on Nanostructures (ICNS8), Sharif University of Technology, Tehran, 18 November 2020.

9- H. Pirdadeh Beyranvand, Z. Tavangar, “Structural and electronic properties of F-decorated γ-Bnyne”, Proceeding of 11th International Chemical Engineering Congress & Exhibition, Iranian Association of Chemical Engineering, Fuman, 28 October 2020.

10- Z. Tavangar, Z. Haji Ahmadi, “Electronic, magnetic and optical properties of Cr,S co-doped zinc oxide for photovoltaic and solar cell application”, Proceeding of 5th International Conference On Recent Innovations Chemistry and Chemical Engineering, Allameh Tabataba'i University, Tehran, 2 February 2018.

11- Z. Tavangar, Z. Haji Ahmadi, “Electronic Properties of (Cr-S) Co-doped Anatase TiO_2 Nanoparticle; A DFT Study”, Abstract Booklet of the Seventh International Conference on Nanostructures (ICNS7), Sharif University of Technology, Tehran, Feb 27-Mar 01, 2018.

12- Z. Tavangar, Z. Haji Ahmadi, “Van der Waals interaction of nitrobenzene with Pd (111)”, Proceeding of 20th Iranian Physical Chemistry Conference, Arak University, Karaj, 20-22 August 2017.

13- Z. Tavangar, H. Basharnavazi, “Theoretical study of non-covalent adsorption of thiophene on boron nitride nanotubes”, Proceeding of 6th International Conference on Nanoscience and Nanotechnology, Kharazmi University, Karaj, 26-28 October 2016.

14- F. Kolahdouzan, Z. Tavangar, H. Kolahdouzan, “Physical Properties Of The Ambient Pressure Dried Silica Nanoporous Aerogel By The Co-Precursor Method”, Proceeding of 19th Iranian Physical Chemistry Conference, University of Guilan, Ziba kenar, 13-15 September, 2016.

15- Z. Tavangar, H. Basharnavaz, “Investigation of the interaction of furan molecule with (9, 0) boron nitride nanotubes”, Proceeding of The Second International Conference in New Researcch on chemistry & chemical engiineeriing, Amirkabir University of Technology, Tehran, 5 April, 2016.

16- Z. Tavangar, P. Mehdizadeh, M. Hamadanian, “Photocatalyst N-doped titanium oxide nanoparticles: Fabrication, characterization, and investigation of the effect of doping on methyl orange dye degradation”, Proceeding of The 9th International Chemical Engineering Congress & Exhibition (IChEC 2015), Shiraz, 26-28 December, 2015.

17- Z. Tavangar, N. Zareie, “DFT studies on the electronic structures of TTA dyes for dye-sensitized solar cells”, Proceeding of The Second Conference on Computational Group Theory, Computational Number Theory and Applications, University of Kashan, Kashan, 13-15 October, 2015.

18- M. Malmir, B. Khoshnevisan, Z. Tavangar, “Carbon nanotubes as lithium storage anode materials: A molecular dynamic simulation”, Proceeding of The Annual Physics Conference of Iran, Sistan and Baluchestan University, Zahedan, 8-11 September, 2014.

19- Z. Tavangar, P. Nekouhesh, “DFT study on the interaction of $B_{24}N_{24}$ nanocage with picoplatin as a anticancer drug”, Proceeding of The Second Conference on Computational Group Theory, Computational Number Theory and Applications, University of Kashan, Kashan, 13-15 October, 2015.

20- Z. Tavangar, M. Hamadanian, H. Basharnavaz, “Modification of conductive properties of (5, 0) and (7, 0) Boron Nitride nanotubes (BNNTs) by Li adsorption”, Proceeding of The Second Conference on Computational Group Theory, Computational Number Theory and Applications, University of Kashan, Kashan, 13-15 October, 2015.

۲۱- مسعود همدانیان، زهرا توانگر، سارا ناصح، "جذب مولکول بنزن بر روی نانولوله کربنی تک دیواره زیگزاگ اکسید شده"، کتابچه یازدهمین همایش شیمی پیام نور، دانشگاه پیام نور، اصفهان، ۲۵-۲۴ اردیبهشت‌ماه ۱۳۹۳.

۲۲- زهرا توانگر، شیوا جهانگیری، "بررسی و مطالعه نظری نانومخروط بورنیتریدی عامل دارشده با مولکول فوران"، کتابچه یازدهمین همایش شیمی پیام نور، دانشگاه پیام نور، اصفهان، ۲۵-۲۴ اردیبهشت‌ماه ۱۳۹۳.

۲۳- زهرا توانگر، اکرم پیوند، "مطالعه عاملدار کردن نانومخروط بورنیتریدی با مولکول پیرول به روش محاسباتی"، کتابچه یازدهمین همایش شیمی پیام نور، دانشگاه پیام نور، اصفهان، ۲۵-۲۴ اردیبهشت‌ماه ۱۳۹۳.

۲۴- مسعود همدانیان، زهرا توانگر، بنفشه نوری، "مطالعه خواص الکترونی نانولوله آلوهینیوم نیتریدی تک دیواره(۸،۰) آلاییده با فلز منیزیم با روش تئوری تابعیت چگالی"، کتابچه یازدهمین همایش شیمی پیام نور، دانشگاه پیام نور، اصفهان، ۲۵-۲۴ اردیبهشت‌ماه ۱۳۹۳.

۲۵- زهرا توانگر، مسعود همدانیان، هادی بشرنواز، "بررسی خواص الکترونی و ساختاری نانولوله‌های بورنیتریدی خالص و ناخالص شده با سزیم"، کتابچه کنفرانس بین‌المللی یافته‌های نوین پژوهشی در علوم شیمی و مهندسی شیمی، تهران،۲۶ شهریورماه ۱۳۹۴.

26- M. Hamadanian, Z. Tavangar, B.Noori, “A Theoretical Study of the Cesium stom Adsorption onto (10,0) Carbon Nanotube”, Proceeding of The 16th Iranian Physical Chemistry Conference, University of Mazandara, Babolsar, 29-31 October, 2013.

27- Z. Tavangar, M. Mohammad, “Molecular Dynamic Simulation of Amino Acids Interaction with Zigzag Boron Nitride Nanotube”, Proceeding of The 16th Iranian Physical Chemistry Conference, University of Mazandara, Babolsar, 29-31 October, 2013.

28- Z. Tavangar, Z. Taherian Arani, “Computational Study on the Glycine And Alanine Interactions with Boron Nitride NanoCone and Platinated Boron Nitride NanoCone”, Proceeding of The 16th Iranian Physical Chemistry Conference, University of Mazandara, Babolsar, 29-31 October, 2013.

29- B. Khoshnevisan, Z. Tavangar, M. Rahimi, M. Yazdani, “Molecular dynamic simulation of Hydrogen physisorption on Si-doped carbon nanotube”, Proceeding of the Annual Physics Conference of Iran, Urmia, 5-8 September 2011.

30- B. Khoshnevisan, Z. Tavangar, M. Yazdani, M. Rahimi, “Investigation the effect of chairality, radius and temperature on Hydrogen physisorption in single and double walled carbon nanotube”, Proceeding of the Annual Physics Conference of Iran, Urmia, 5-8 September 2011.

31- B. Z. Tavangar, Khoshnevisan, M. Yazdani, M. Rahimi, “The role of thermostat in the simulation of carbon nanotubes”, Proceeding of The 14th Iranian Physical Chemistry Conference, University of Tehran, kish, 25-28 February 2011.

32- H. Sabzyan, Z. Tavangar, “A computatuonal study of molecular transport through carbon nanotube”, Proceeding of The 13th Irainian Physical Chemistry Seminar, Shiraz, Iran, April 12-15, 2010.

33- H. Sabzyan, Z. Tavangar, “Molecular Dynamic Simulation Of The Flow Of The CO/CO_2 Gases Through Carbon Nanotube Junction”, *Proceeding of The Forth Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 12-15 July 2010*.

34- Z. Tavangar, M. Hamadanian, A. R. Ashrafi, H. Sabzyan, “Symmetry of Capped Nanotube”, *Proceeding of The First Conference and Workshop on Mathematical Chemistry, Tehran, Iran 29-31 January 2008*

35- Z. Tavangar, A. R. Ashrafi, M. Hamadanian, , H. Sabzyan, “Computing Distance Matrix and Wiener Index of a capped Nanotube”, *Proceeding of The First Conference and Workshop on Mathematical Chemistry*, Tehran, Iran 29-31 January 2008.

36- H. Sabzyan, Z. Tavangar, “Simulation of the He-Ar gas mixture flow model 2-D CNT with different (**n**, **m**)”, *Proceeding of The 41th IUPAC World Chemistry Congress* , Torino, Italy, 5-11 August 2007.