In The Name of God, The Compassionate, The Merciful

Curriculum Vitae

A) Personal Information

Name: Hassan Sabzyan
Nationality: Iranian
Date of Birth: December 19th, 1965 (Abadan, Khuzestan)
Address: Department of Chemistry, University of Isfahan, Isfahan 81746-73441, I. R. Iran
Phone: 98 - 31 - 3793 4916, 793 4900 (secretary)
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Academic Status: Professor of Physical Chemistry (Since 2011)

B) Educations

1980 – 1983 High School (Mathematics and Physics)
17th Shahrivar High School, Sari, Mazandaran, Islamic Republic of Iran

1984 – 1987 Bachelor of Science (BSc) in ChemistryUniversity of Isfahan, Isfahan 81746-73441, Islamic Republic of Iran

1987 – 1991 Master of Science (MSc) in Physical Chemistry
Thesis Title: Order-Disorder in Mixtures of Alkali and Alkaline Earth Feldspars.
Supervisor: Gh. Parsafar (Professor of Physical Chemistry at Sharif University of Technology)
University of Isfahan, Isfahan 81746-73441, Islamic Republic of Iran

1993 – 1997 Doctor of Philosophy (PhD) in Physical Chemistry
Thesis Title: A Combined Experimental and Theoretical Study of NMR Spin-Lattice Relaxation
Times in HD-Ar and D₂-Ar Mixtures.
Supervisors: Professors F. R.W. McCourt and W. P. Power,
University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

C) Research Interests

1. Electric and Magnetic Properties of Molecules and Nano-size Materials.

(Nano-electronics, Nano-optics, Solid State Devices)

- 2. Computational Physics and Chemistry, Simulation and Molecular Modeling and Design.
- 3. Laser Spectroscopy and Interaction of Ultrashort Intense Laser Fields with Matter
- 4. Molecular Transport Properties and Relaxation Phenomena in the Gas Phase.
- 5. Chemical Kinetics and Reaction Dynamics.
- 6. NMR Spectroscopy.
- 7. Spectroscopy and Electrochemistry of Single Crystals and Self-Assembled Monolyers.

D) Practical Skills and Experiences

1. Establishment of gas phase NMR experiments in the University of Waterloo (Canada) and successful relaxation time measurements on several gas phase samples including different isotopic hydrogen-argon mixtures.

2. Experience with NMR instruments and measurements, and familiarity with pulse programming for BRUKER NMR instruments.

3. Extensive experience with close-coupled (CC) calculations of the scattering cross sections using programs MOLSCAT and SBE.

4. Experience with DOS/WINDOWS/UNIX/LINUX computer operating systems and their related softwares, and writing c-shell scripts in UNIX/LINUX environment.

5. Extensive experience with FORTRAN-77 and familiarity with C and C++ scientific programming, familiarity and experience with MAPLE and MATLAB softwares.

6. Experience with molecular modeling, molecular dynamic simulations, and *ab initio* and *semiempirical* calculations (molecular structures and properties, interpretations) using softwares such as DL_POLY, GRPMACS, Gaussian and HyperChem.

7. Studies and thoughts in fundamental aspects of laser-molecule and laser-atom interactions.

8. Familiarity and experiences with UV-VIS, FT-IR, XRF Spectrometers, and SC-XRD.
 9. Familiarity and experience with SPM (AFM, MFM, STM), SEM and TEM Techniques.
 10. Experiences in purchasing/evaluation of scientific/industrial instruments/equipments.

E) Teaching Experiences

Undergraduate Courses:

Quantum Chemistry I, Molecular Spectroscopy, Physical Chemistry-I and II, Physical Chemistry Lab-I and -II, General Chemistry-I and -II, and Biophysical Chemistry.

Graduate (MSc and PhD) Courses:

Quantum Chemistry II and III, Molecular Spectroscopy II and III, NMR Spectroscopy, Chemical Kinetics and Reaction Dynamics, Computational Quantum Chemistry, Non-Equilibrium Statistical Mechanics, Irreversible Thermodynamics, Molecular Modeling, Quantum and Computational Molecular Biology, Fundamentals of NanoScience, Solid State Physical Chemistry.

F) PhD Theses Supervised

- **1.** Ab initio study of the F_2 - F_2 interaction potential energy surface and calculation of some transport properties of the F_2 gas.
- (Dr. Mohammad-Reza Noorbala, University of Isfahan, August 2003)
- **2.** Theoretical study of the ionization rates of H_2^+ and D_2^+ molecular ions in ultra-short intense laser fields.
- (Dr. Mohsen Vafaee, Tarbiat Modares University, December 2004).

3. Theoretical design and computational characterization of multipole molecular switches. (Dr. Davood Farmanzadeh, University of Isfahan, August 2006).

- **4.** Characterization of the flow of the CO/CO₂ gases through carbon nanotube junctions using molecular dynamic simulations.
- (Dr. Z. Tavangar, University of Isfahan, September 2009)

5. Theoretical study of the interaction of ultra-short intense laser fields with two-electron H_2 system.

(Miss. Behnaz Buzari, University of Isfahan, 2013, Co-supervised by Dr. Vafaee)

6. Theoretical and computational study of the Peltier effect in molecular nanoelectronic systems. (Mr. Reza Safari-Sichani, University of Isfahan, 2013).

7. Theoretical study of the magnetic interaction of ultra-short intense laser fields with H₂⁺ and D₂⁺ molecular ions.
(Mr. Hossein Ebadi, University of Isfahan, 2004, *discontinued*).

8. Potential energy curves and spectroscopic properties of diatomic dianions.(Miss. Zeinab Noorisafa, University of Isfahan, 2013)

9. Potential energy curves and spectroscopic properties of diatomic dications.(Mrs. Elham Keshavarz, University of Isfahan, 2014)

10. Evolution of electron wavefunction during electron transfer process (Mr. Mohammad Jafar Jenabi, University of Isfahan, 2011, in progress)

11. Computational study of charge distribution in neighboring grapheme sheets. (Mrs. Nargess Sadeghpour, University of Isfahan, 2012, *in progress*)

12. Evolution of two-electron density(Mr. Yusof Korrani, University of Isfahan, 2013, in progress)

13. Forward scattering in the interaction of ultrashort intense laser pulses with H_2^+ system. (Miss. Fatemeh Gheisi, University of Isfahan, 2015, in progress)

14. Preparation and computational studies on a couple of new optodes for iron(III)(Mr. Mohsen Movahedi, 2014 in progress), (Co-supervising with Dr. AliReza Firouz)

G) MSc Theses Supervised

Theoretical analysis and simulation of J-coupling multiplet collapse of ¹H-NMR spectrum of HD in the HD-Ar gas mixtures, and Its Temperature Dependence.
 (Mrs. Anahita Saadatmand, University of Isfahan, January 1999)

2. *Ab initio* study of physical and chemical properties of pure and He-, Li- and Ne-doped graphite.

(Miss. Masumeh Afiati, University of Isfahan, August 2000)

3. *Ab initio* study of physical and thermochemical properties of helium clusters. (Mrs. Farzaneh Zanjanchi, University of Isfahan, August 2000)

4. Experimental and theoretical study of the kinetics and dynamics of sodium-water reaction and their correlation.

(Mr. Mohsen Bahmani, University of Isfahan, August 2000)

5. Bloor, a sofware for determining crystalline structures from X-ray diffraction data. (Mrs. Marzieh Kasaei, University of Zanjan, June 2001)Co-supervised by Dr. Ali Asghar Torabi

6. *Ab initio* and DFT study of one- and two-dimensional lithium lattices. (Miss. Fakhrossadat Mohammadi, University of Isfahan, June 2002)

7. *Ab initio* study of the structure, thermochemical and spectroscopic properties, and possibility of non-adiabatic crossing between potential energy curves of two internal motions of the 2-hydroxy-4-phenyl-2,4-cyclopentadien-1-one (HPCP) molecule.
(Mr. Afshin Abbassi, University of Isfahan, September 2002)
Advised by Professor Majid MirMohammad Sadeghi

8. Ab initio study of some oxiranes and thiiranes, and the kinetics and mechanism

of the oxirane \rightarrow thiiranes reactions.

(Mr. Mohammad-Hossein Ghaderi-Moghaddam, University of Isfahan, August 2003) Co-supervised by Professor Iraj Mohammadpour Baltork

9. Theoretical study of the kinetics and mechanism of the pyrolysis of methane on the graphite Surface.

(Mr. Mohammad-Bagher Moheb-Ali, Ferdowsi University of Mashhad, February 2003) Co-supervised by Professor Seyyed Faramarz Tayyari

10. Semiempirical and molecular dynamics study of the pyrolysis of methane on the graphite surface.(Miss. Mahnaz Babajani, University of Lorestan, September 2003)Co-Supervised by Dr. Reza Sadeghi Sarabi

11. Molecular dynamics and NMR study of the orientation of small solutes in Water.(Miss. Razieh Amiri, University of Isfahan, June 2004)

12. Contribution of vibrational motion to NMR shielding constants (and line-shapes).(Miss. Behnaz Buzari, University of Isfahan, June 2005)

13. Ab initio study of intramolecular oxygen exchange in some heterocyclic compounds. (Mrs. Mojgan Mokhtari, University of Yazd, September 2005)Co-Supervised by Dr. Mohammad Reza Nourbala

14. Theoretical and computational study of the optical rotation of small molecules containing one and two chiral centers.

(Miss. Fariba Taghavi, University of Isfahan, October 2005)

15. Synthesis and characterization of copper quantum dots based on alumina template.(Mr. AbdolReza HajHashemi, University of Isfahan, November 2008)Co-Supervised by Dr. Reza Karimi Shervedani

16. Design and ab initio characterization of a family of di- and tri- substituted benzene cores as potential quantum dots for nanocircuit devices.

(Miss. Zeinab Noorisafa, University of Isfahan, September 2008)

17. Computational study of the formation and addition reactions of benzyne.(Miss. Sedigheh Hosseini, Payam-Noor University of Ardakan, February 2008)Advised by Dr. Reza Behjatmanesh Ardakani

18. Computational study of the characteristics of CdSe nanoparticles and their size-dependence.(Mrs. Hoda Iravanizadeh, Payam-Noor University of Shiraz, March 2009)Co-Supervised by Dr. Masoud Kavosh Tehrani

19. Synthesis and QSAR study of some 4-heteroaryl-2,6-dimethyl-3,5-bis-N-phenyl(pyridyl)-1,4-dihydropyridin derivatives having pharmaceutical effects.
(Miss. Fatemeh Safari, Medical University of Isfahan, August 2010)
Co-Supervised by Dr. Afshin Fasihi and Dr. Farshid Hassanzadeh

20. Density functional theory study of the charged adamantanes and sila-adamantanes.(Miss. Behnaz Saed, University of Isfahan, September 2010)

21. A new Index for the description of the asymmetry of the electron density. (Miss. Nargess Sadeghpur, University of Isfahan, September 2010)

22. Molecular Dynamics Simulation of the diffusive flow inside carbon nano-tori.(Miss. Samira Gholami, University of Isfahan, September 2010)

23. Molecular dynamics simulation study of lithium carbides.(Miss. Hajar Nematollahi, University of Isfahan, October 2010)

24. Computational study of the effects of fluorination on the physicochemical properties of 3-hydroxypyridinones.

(Dr. Danial Shamshirian, Medical University of Isfahan, Dept. of Pharmacy, February 2010). Co-Supervised by Dr. Lotfollah Saghaee Dehkordi

25. Molecular dynamics simulation study of the scattering of Ne and Ar from SiC surface. (Miss. Arezu Dehbashi, University of Isfahan, October 2010)

26. Evolution of free electron wavepacket to bound electron wavefunction.(Miss. Fatemeh Alavi, University of Isfahan, July 2011), Advised by Dr. Mohsen Vafaee

27. Evolution of the two-dimentional H_2^+ electron and nuclear wavepackets under magnetic and electric fields of ultrashort intense laser pulse.

(Mr. Hamed Ahmadi, University of Isfahan, July 2011), Advised by Dr. Mohsen Vafaee.

28. Molecular dynamics simulation of diffusion phenomena through polymer-clay nanocomposites films.

(Mr. Amir-Hossein HajiAlirezaee, University of Isfahan, September 2011)

Co-Supervised by Dr. Amir-Hossein Navarchian.

29. Synthesis and QSAR MLR study on 3-hydroxypyrimidinon anti-malaria drugs.(Dr. HamidReza Sakhi, Faculty of Pharmacy, Isfahan University of Medical Science, 2012)Co-Supervised by Dr. Lotfollah Saghaee.

30. Kinetics and dynamics of diffusive dissolution of NaOH and KOH in water. (Miss. Maryam SeyyedSharifi, 2013)

31. Computational Study of Oxyluciferine.(Miss. Faezeh Seddighi, 2014)

32. Molecular dynamic simulation of the vibration of Silicon carbide nanotubes.

(Miss. Maryam Ramazani, 2014)

33. Investigation of the activity of the self-assembled monolayer of Glucose oxidase on the gold surface using STM method.

(Mr. Abbass Derakhshan, 2014)

34. Reactive molecular dynamic simulation of the formation of fume silica. (Mr. Ebrahim Izadi, 2015)

35. Kinetic modeling of the formation of fume silica. (Mr. Farhad Ghalami, 2015)

36. Quantum dynamics of free electron capture.(Mrs. Nasrin Sadeghi, in progress)

37. Molecular dynamics simulation of the flow of a gas mixture in graphene oxide (Mr. Meisam Hadian, in progress)

38. Synthesis and computational studies on NiCo₂O₄ as photocatalyst.
(co-supervised by Emeritus Professor Habibi)
(Mr. Mojtaba Beiranvand)

H) MSc and PhD Theses Advised

1. Calculation of EFGs and NQR frequencies of ¹⁴N in two polycyclic aromatic compounds using ab initio calculations.

Mr. Nasser Zamand, March 2002.

Supervisor: Professor Nasser L. Hadipour, Tarbiat Modares University.

2. Photocatalytic ring opening of α -epoxy ketones in the presence of different nucleophiles Dr. Farzad Nikpour, December 2001.

Supervisor: Professor HamidReza Memarian, University of Isfahan.

3. Calculation of structure factor and surface tension of liquid alkali metals using LIR and DSEOS.Mr. Reza Safari Sichani, September 2003.Supervisor: Dr. Nahid Farzi, University of Isfahan.

4. A dynamics investigation of H abstraction reaction of OH radical and CH₃CHF₂.
Mr. Mehdi Taghikhani, January 2005.
Supervisor: Professor Gholam-Abbass Parsafar, Sharif University of Technology.

5. Stereoelectronic effects on the structure, energetic and reactivity of some organic compounds. Dr. Sattar Arshadi, October 2005.

Supervisor: Professor Mohammad Zaman Kassaee, Tarbiat Modares University.

6. Theoretical and Fluorescence study of some Aflatoxins, and their determination using multilinear regression analysis.

Dr. Mohammad Aghamohammadi, January 2007.

Supervisor: Professor Nader Alizadeh, Tarbiat Modares University.

7. Oxidation of some dihydropyrimidinones under thermal condition, and UV-Vis, ultrasonic and microwave irradiations.

Dr. Asadollah Farhadi, September 2009.

Supervisor: Professor HamidReza Memarian, University of Isfahan.

8. Investigation of liquid-liquid phase equilibria in aqueous systems using Monte-Carlo simulations.

Miss. Mitra Hajipur, July 2009.

Supervisors: Dr. Seyyed Foad Aghamiri and F. Seyedeyn-Azad, University of Isfahan.

9. Immobilization of bronic and hydroxamic acid functionalized surfaces on gold via in-situ layerby-layer functionalization of self-assembled monolayers: preparation, electrochemical characterization and application,

Dr. Mojtaba Bagherzadeh, September 2009.

Supervisor: Dr. Reza Karimi Shervedani, University of Isfahan.

10. Synthesis and oxidation of some new 2-oxo-1,2,3,4-tetrahydropyrimidin-5-carboxamides under thermal conditions, ultrasound, microwave, and ultraviolet irradiations.

Dr. Musa Soleymani, February 2011.

Supervisor: Professor HamidReza Memarian (Department of Chemistry, University of Isfahan)

11. DFT and TD-DFT investigation of physical and chemical properties of azo/hydrazone dyes adsorbed on the cellulose fibers.

Dr. Farzaneh Zanjanchi, February 2011

Supervisor: Professor Nasser L. Hadipour, Tarbiat Modares University.

12. Preparation and study of new molecular nanostructures on the gold surface based on in-situ and ex-situ ferrioxamation using CV, SWV, EIS and STM techniques.Dr. Zakieh Akrami, October 2012Supervisor: Professor Reza Karimi Shervedani

13. Simulation of adsorption from air flown over a zeolite bed using lattice Boltzmann method.Dr. Mahdi Rahmani Gurtani, PhD, March 2013Supervisor: Professor Mahmood Ashrafizadeh (Isfahan University of Technology)

14. Experimental and modeling study of adsorption of heavy metals by γ-alumina nanoparticlesMrs. Maliheh Fouladgar, MSc, November 2012.Supervisor: Dr. Masoud Beheshti (Chemical Engineering, University of Isfahan)

15. Experimental measurements and predictions of the size distribution of water droplets in wateroil emulsions. Mr. Arash Amani, MSc, February 2014.

Supervisor: Dr. AliReza SoleimaniNazar (Chemical Engineering, University of Isfahan)

16. A Mont-Carlo simulation study of adsorption of CO₂ and SO₂ gases on carbon nanotube and graphene.

Mrs. Zahra Nickmand, PhD, November 2013.

Supervisor: Dr. Seyyed Foad Aghamiri (Chemical Engineering, University of Isfahan)

I) Publications

86. Amir H. Haji Alirezaie, Amir H. Navarchian, and Hassan Sabzyan.
Molecular dynamics simulation of gas diffusion in polyethylene-clay nanocomposites with different silicate layers configurations
Polymer Sciences A, 58, 487-498 (2016).

85. Hassan Sabzyan and Nargess Sadeghpour"Importance of Unit Cells in Accurate Evaluation of the Characteristics of Graphene"Zeitschrift für Naturforschung A, 71, 315 (2016)

84. Hassan Sabzyan and Mohammad Jafar Jenabi"Electron quantum dynamics in atom-ion interaction",J. Chem. Phys. 144, 134306 (2016);

83. Masoud Beheshti, Maliheh Fouladgar, Hassan Sabzyan,
"Single and binary adsorption of nickel and copper from aqueous solutions by γ-alumina nanoparticles: Equilibrium and kinetic modeling"
Journal of Molecular Liquids, 211, 448-456 (2015).

82. Mohammad Mahmoudzadeh, Afshin Fassihi, Farid Dorkoosh, Reyhaneh Heshmatnejad, Karim Mahnam, Hassan Sabzyan, Amir Sadeghi

"Elucidation of Molecular Mechanisms Behind the Self-Assembly Behavior of Chitosan Amphiphilic Derivatives through Experiment and Molecular Modeling" Pharmaceutical Research 32, 3899-3915 (2015).

81. Mohammad Sadegh Sadeghi Googheri, Mohammad Reza Housaindokht, Hassan Sabzyan "Theoretical studies on the deacylation step of acylated Candida Antarctica lipase B: Structural and reaction pathway analysis" Journal of Molecular Graphics and Modelling 57, 9-19 (2015)

80. Reza Karimi Shervedani, Zeinab Rezvaninia, Hassan Sabzyan

"Oxinate-Aluminum (III) Nanostructure Assemblies Formed via In-situ and Ex-situ Oxination of Gold-Self-Assembled Monolayers Characterized by Electrochemical, Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy, and X-ray Photoelectron Spectroscopy Methods"

Electrochimica Acta 180, 722-736 (2015)

79. Hassan Sabzyan, Elham Keshavarz and Zeinab Noorisafa
"Evaluation of the B3LYP and HSE06 density functionals in the calculation of spectroscopic properties of the HCl²⁺ dication"
Journal of Iranian Chemical Society, 12 (2015) 581–586.

78. Elham Keshavarz, Hossein Farrokhpour, Hassan Sabzyan, Zeinab Noorisafa, Antti Kivimäki and Robert Richter

Core photoionization of the argon dimer in the 255–340-eV photon-energy range studied by a photoelectron-photoion-photoion coincidence technique.

Physical Review A 89 (2014) 053409.

77. Mohammad Sadeghi Googheri, Mohammad Reza Housaindokht, Hassan Sabzyan "Reaction mechanism and free energy profile for acylation of Candida Antarctica Lipase B with Methylcaprylate and Acetylcholine; Density functional theory calculations" Journal of Molecular Graphics and Modelling 54, 131-140 (2014)

76. Hassan Sabzyan, Narges Sadeghpour

A Minimum Asymmetry Index for Measuring Asymmetry of the Electron Density Distribution. MATCH (Communications in Mathematical and in Computer Chemistry) 72 (2014) 359-373.

75. Zahra Nickmand, Seyed Foad Aghamiri, Mohammad Reza Talaie Khozanie and Hassan Sabzyan

"A Monte Carlo Simulation of the Adsorption of CO₂ and SO₂ Gases in Pure and Functionalized Single Walled Carbon Nanotubes"

Separation Science and Technology 49 (2014) 1–7.

74. H. Ahmadi, A. Maghari, H. Sabzyan, A. R. Niknam, and M. Vafaee "Effect of nuclear motion on high-order-harmonic generation of H_2^+ in intense ultrashort laser pulses"

Physical Review A 90, 043411 (2014).

73. Hassan Sabzyan, Seyyed Hamed Ahmadi and Mohsen Vafaee
High-order harmonic generation by H₂⁺ in super-intense xuv ultrashort laser pulses.
J. Phys. B: At. Mol. Opt. Phys. 47 (2014) 105601.

72. Zeinab Noorisafa, Hassan Sabzyan, Elham Keshavarz
Metastable excited states of OBr²⁻ and OCl²⁻ dianions.
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 132 (2014) 672-677.

71. Narges Yaghoobi Nia, Pooria Farahani, Hassan Sabzyan*, Mahmoud Zendehdel and Mohsen Oftadeh

A combined computational and experimental study of the $[Co(bpy)_3]^{2+/3+}$ complexes as oneelectron outer-sphere redox couples in dye-sensitized solar cell electrolyte media. Phys. Chem. Chem. Phys. 16 (2014) 11481. **70.** Reza Karimi Shervedani, Zeinab Rezvaninia, Hassan Sabzyan, Hassan Zali Boeini Characterization of gold-thiol-8-hydroxyquinoline self-assembled monolayers for selective recognition of aluminum ion using voltammetry and electrochemical impedance spectroscopy. Analytica Chimica Acta 825 (2014) 34-41.

69. Hassan Sabzyan and Fariba TaghaviTheoretical study of magnetic susceptibility and optical activity of small molecules containing one chiral center.Physical Chemistry Research 2 (2014).

68. Hassan Sabzyan, Zeinab Noorisafa, Elham Keshavarz
Ground and excited states of the diatomic dianion Cl₂^{2–}.
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 117 (2014) 95-101.

67. Hassan Sabzyan, Elham Keshavarz and Zeinab Noorisafa A review article titled "Diatomic dications and dianions". Journal of Iranian Chemical Society, 11 (2013) 871-945.

66. Zahra Nickmand D. D. Do, D. Nicholson, Seyed Foad Aghamiri, Mohammad Reza Talaie Khozanie and Hasan Sabzyan"GCMC simulation of argon adsorption in wedge shaped mesopores of finite length"Adsorption 19 (2013) 1245–1252.

65. Hossein Tavakol and Hassan Sabzyan Possibility of non-adiabatic level crossing by DFT study of tautomerism and potential energy surfaces in of 3-hydroxy-5-(pyrimidin-2-yl)-2H-pyrrol-2-one and its tautomer. Journal of Physical Organic Chemistry, 24 (2011), 414-422.

64. Reza Safar and Hassan Sabzyan

Detailed mapping of intramolecular energy transfer in field-effect single-molecule nanoelectronic devices.

Journal of Iranian Chemical Society, (2014).

63. Hassan Sabzyan and Behnaz SaedComputational study of adamantanes using floating basis functionsStructural Chemistry 25 (2014) 1207-1216.

62. Behnaz Buzari, Mohsen Vafaee, Hassan Sabzyan
"High harmonic generation from pre-ionized H₂ in ultrashort intense laser fields."
Journal of Physics B. Atomic, Molecular and Optical Physics 46 (2013) 245401.

61. Hamid R. Memarian, Hassan Sabzyan & Mahnaz Ranjbar "DFT study of 1-, 4-, and 5-substituted 2-oxo-1,2,3,4-tetrahydropyrimidines: substituent steric and electronic effects, and ring flipping" Structural Chemistry 25 (2014) 85-94.

60. Reza Safari and Hassan Sabzyan"Detailed mapping of intramolecular energy transfer in field-effect single-molecule nanoelectronic devices"Journal of the Iranian Chemical Society 11 (2014) 1513-1532.

59. Farzaneh Zanjanchi, Nasser L. Hadipour, Hassan Sabzyan and Javad Beheshtian "Theoretical investigation of azo dyes adsorbed on cellulose fibers: 2. Spectroscopic study"

58. Farzaneh Zanjanchi, Nasser L. Hadipour, Hassan Sabzyan and Javad Beheshtian Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures.

Journal of the Iranian Chemical Society 10 (2013) 985–999

Journal of the Iranian Chemical Society 11 (2014) 111–121.

57. Hamid Reza Memarian, Mahnaz Ranjbar, Hassan Sabzyan, Mohammad Hossein Habibi, and Takayoshi Suzuki
"Molecular structure and conformational analysis of two 2-oxo(thioxo)1,2,3,4-tetrahydropyrimidine-5-esters"
Journal of Molecular Structure 1048 (2013) 196–201

56. Hamid R. Memarian, Mahnaz Ranjbar, Hassan Sabzyan and Abolfazl Kiani Substituent effects on the voltammetric studies of 2-oxo-1,2,3,4-tetrahydropyrimidines Comptes Rendus Chimie, 15 (2012) 1001–1011

55. Hassan Sabzyan and Behnaz SaedComputational study of aza-adamantanes as multivalent bases.Structural Chemistry 23 (2012) 1971-1979.

54. Lotfollah Saghaie, Hamidreza Sakhi, Hassan Sabzyan, Mohsen Shahlaei and Danial Shamshirian

Stepwise MLR and PCR QSAR study of the pharmaceutical activities of antimalarial 3hydroxypyridinone agents using B3LYP/6-311++G** descriptors. Medicinal Chemistry Research, 7 (2012) 1-10.

53. Electrochemical probe of natural DNA attached onto the gold–thiol SAMs via Zr(IV) ion glue. Reza Karimi Shervedani, Sima Pourbeyram, Hassan Journal of Electroanalytical Chemistry, 660 (2012) *37-44*.

52. HamidReza Memarian, Mousa Soleymani and Hassan Sabzyan Light-induced dehydrogenation of 2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxamides. Journal of the Iranian Chemical Society, 9 (2012) 805-813.

51. Mohsen Vafaee, Firoozeh Sami, Babak Shokri, Behnaz Buzari, and Hassan Sabzyan Precise description of single and double ionization of hydrogen molecule in intense laser pulses. Journal of Chemical Physics, 137 (2012) 044112.

50. Behnaz Buzari, Mohsen Vafaee, Hassan Sabzyan
Mapping electron dynamics in molecular H₂ using high-order-harmonic-generation time profiles.
Physical Review A, 85 (2012) 033407.

49. Hassan Sabzyan and Reza SafariIntramolecular thermoelectric-like effects in field-effect molecular nanoelectronic devices.Europhysics Letters, 99 (2012) 67005.

48. Reza Karimi Shervedani, Zakyeh Akrami, Hassan Sabzyan Nanostructure molecular assemblies constructed based on ex-situ and in-situ layer-by-layer Ferrioxamation characterized by electrochemical and scanning tunneling microscopy methods. Journal of Physical Chemistry C, 115 (2011) 8042-8055.

47. Farzaneh Zanjanchi, Nasser L. Hadipour, Hassan Sabzyan, Javad Beheshtian "Photo-oxidation of phenylazonaphthol dyes and their reactivity analysis in the gas phase and adsorbed on cellulose fibers states using DFT and TD-DFT" Dyes and Pigments 89 (2011) 16-22.

46. HamidReza Memarian, Mousa Soleymani, Hassan Sabzyan, Mojtaba Bagherzadeh and Hamed Ahmadi

"Voltammetric oxidation of 2-oxo-1,2,3,4-tetrahydropyrimidin-5-carboxamides: substituent effects."

Journal of Physical Chemistry A, 115 (2011) 8264-8270.

45. Mitra Hajipour, Seyyed Foad Aghamiri, Hassan Sabzyan, Fakhri Seyedeyn Azad Extension of the exp-6 model to the simulation of vapor-liquid equilibria of primary alcohols and their mixtures.

Fluid Phase Equilibria, 301 (2011) 73-79.

44. Farzaneh Zanjanchi, Nasser L. Hadipour, Hassan Sabzyan, Javad Beheshtian

Photo-oxidation of phenylazonaphthol dyes and their reactivity analysis in the gas phase and adsorbed on cellulose fibers states using DFT and TD-DFT. Dyes and Pigments 89 (2011) 16-22.

43. HamidReza Memarian, Hassan Sabzyan, Assadollah Farhadi DFT study of the molecular structure of 3,4-dihydropyrimidin-2(1H)-ones. Monatshefte Fur Chemie, 141 (2010) 1203-1212.

42. HamidReza Memarian, Assadollah Farhadi, Hassan Sabzyan, Mousa Soleimani
Photo-oxidation of 5-acetyl-3,4-dihydropyrimidin-2(1H)-ones.
Journal of Photochemistry and Photobiology A – Chemistry, 209 (2010) 95-103.

41. HamidReza Memarian, Assadollah Farhadi, Hassan Sabzyan Ultrasound-assisted dehydrogenation of 5-acetyl-3,4-dihydropyrimidin-2(1H)-ones Ultrasonics Sonochemistry, 17 (2010) 579-586.

40. Hossein Ebadi, Hassan Sabzyan Evolution of the H_2^+ electron wavepacket under magnetic and electric fields of ultrashort intense laser pulse. Journal of The Iranian Chemical Society, 6 (2009) 489-503.

39. Hassan Sabzyan, Hossein Ebadi Ionization of a 1-D model of H_2^+ from different states in intense laser fields. Iranian Journal of Science and Technology A, 33 (2009) 87-102.

38. Ali Reza Ashrafi, Masoud Hamadanian, Zahra Tavangar, Hassan Sabzyan, Symmetry of a Capped Nanotube.
Digest Journal of Nanomaterials and Biostructures, 4 (2009) 319 – 322.

37. Hassan Sabzyan, Zahra Tavangar,

Characterization of the flow of the CO/CO_2 gases through carbon nanotube junctions using molecular dynamic simulations.

Chemical Physics, 362 (2009) 120-129.

36. Hassan Sabzyan, Behnaz BuzariTheoretical study of the contribution of vibrational motions to nuclear shielding constants.Chemical Physics 352 (2008) 297–305.

35. H. Loghmani-Khouzani*, H. Sabzyan, A. Rezaei-Pooranari Synthesis and structure of α-azo-2-ketomethylquinolines. Dyes and Pigments, 76 (2008) 447-454.

34. Hassan Sabzyan, Reza Safari,

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28. Hassan Sabzyan, Farzaneh Zanjanchi
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24. Hassan Sabzyan, Farzaneh ZanjanchiA Computational Study of 3-D Helium Clusters.*Journal of the Chinese Chemical Society*, 54 (2007) 843-852.

23. Hassan Sabzyan, Farzaneh ZanjanchiA Theoretical Study of 1-D and 2-D Helium Lattices.*Journal of the Chinese Chemical Society*, 54 (2007) 303-312.

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21. Hassan Sabzyan, Davood FarmanzadehElectric field effects on the performance of a candidate multipole molecular switch, a quantum computational study.Journal of Computational Chemistry, 28 (2007) 922-931.

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17. Hassan Sabzyan, Mehrdad Bamdad,A theoretical study of the bonding structure of carbonyl sulfide (OCS).*Theochem*, 712 (2004) 109-115. (I have retracted this article.)

16. Hassan Sabzyan, Abdollah Omrani

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14. Soheila Javadian, Hassan Sabzyan

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13. Hassan Sabzyan, Mahnaz BabajaniA Semiempirical Quantum Mechanical Study of Methane-Graphite Interaction.*Theochem* 726 (2005) 155-160.

12. K. Khosravi, H. Sabzyan, A. Zeini, G. A. ParsafarA More Accurate Prediction of Liquid Evaporation Flux.Iranian Journal of Chemistry and Chemical Engineering, 23 (2004) 45.

11. Hassan Sabzyan, Hossein NikoofardHalomethylpyrroles as candidate monomers for conducting polymers; A theoretical study.*Chemical Physics*, 306 (2004) 107-115.

10. Mohsen Vafaee, Hassan Sabzyan A detailed and precise study of the ionization rates of H_2^+ in intense laser fields. *Journal of Physics B: At. Mol. Opt. Phys.* 37 (2004) 4143-4157. 9. Hassan Sabzyan, Fakhrossadat MohammadiDFT study of one-dimensional lithium lattices as nanowires.*Chemical Physics*, 301 (2004) 141-152.

8. Hassan Sabzyan, William P. Power, Frederick R. W. McCourt
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7. Hassan Sabzyan, Abdollah Omrani

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6. Hassan Sabzyan, Zahra Kalantar Ab initio RHF and density-functional B3LYP and B3PW91 study of (NPF₂)_n; n=2, 3, 4 and (NPX₂)₃; X=H, Cl, Br cyclic phosphazenes. THEOCHEM, 663 (2003) 149-157.

5. Mohammad-Reza Noorbala, Hassan Sabzyan
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4. Hassan Sabzyan, Mohammad-Reza Noorbala
Basis set effects on the intermolecular interaction of the F₂–F₂ system. *THEOCHEM*, 636 (2003) 185-193.

3. Hassan Sabzyan, Mohammad-Reza Noorbala *Ab initio* and DFT study of carbon monoxide cyclic oligomers, (CO)₂ to (CO)₆. *THEOCHEM*, 626 (2003) 143-158. **2.** Hassan Sabzyan, William P. Power, Frederick R. W. McCourt Proton and Deuteron Spin-Lattice Relaxation Times in HD-Ar Mixtures: A Combined Experimental and Theoretical Study.

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1. Hassan Sabzyan, William P. Power, Frederick R. W. McCourt,

Deuteron Spin-Lattice Relaxation Times in D₂-Ar Mixtures: A Combined Experimental and Theoretical Study.

Journal of Chemical Physics, 108 (1998) 2361-2374.

J) Academic Affairs, and Management Assignments and Activities

1. Vice Chairman of the Department of Chemistry, University of Isfahan (2 years).

2. Teaching Evaluation Committee of the University of Isfahan (10 years).

3. Manager of the Foreign Purchase Department (8 years).

4. Member of the Engineering Sub-Committee of the Promotion Board (Hey'at Momayyezeh) of the University of Isfahan (10 years).

5. Head of the Central Laboratory of the University of Isfahan (2 years).

6. Chairman of the First Student Conference on the "Applications of Chemistry in Industry",2006.

7. Scientific Chairman of "The 10th Physical Chemistry Seminar of Iran", (2007).

8. Member of the Scientific and Executive Committees of a number of Seminars and conferences.

9. Chairman of the Department of Chemistry, University of Isfahan (3 years)

10. Member of a number of university committees (various durations)

K) Oral and Poster Presentations (not updated, about 80 presentations)

1. The First Iranian Workshop on Computational Quantum Chemistry (as lecturer). Department of Chemistry, University of Shiraz, Shiraz, I. R. Iran, August 7-16, 2002.

2. Chemical Oscillations; Theory and Experimental Demonstration. *Invited Speaker, Chemistry Seminar Series, June 1991, Shahid Baahonar University, Kerman, I. R. Iran. (Oral)*

3. Order-Disorder in Mixtures of Alkali and Alkaline Earth Feldspars.

The 7th Iranian Chemistry and Chemical Engineering Conference, September 1-3, 1992, Shahid Montazeri Township Hall, Iranian Oil Company, Isfahan, I. R. Iran. (Oral)

4. Evaluation of Intermolecular Potentials Using NMR: A Spin-Lattice Relaxation Time Study of the HD-Ar System. *MOOT-VIII NMR Symposium*, September 30-October 1, 1995, University of Ottawa, Ottawa, Canada. (Oral)

5. NMR Spin-Lattice Relaxation Study of the HD-Ar System. *The 11th Annual University of Waterloo Symposium on Chemical Physics,* November 3-5, 1995, University of Waterloo, Waterloo, Canada. (Poster)

6. Gas Phase NOE measurement on HD-Ar Gas Mixtures. *MOOT-IX NMR Symposium*, October5-6, 1996, Université Laval, Quebec City, Canada. (Poster)

7. Proton NMR Spin-Lattice Relaxation Times in H₂-Ar Gas Mixtures. *MOOT-XIII NMR Symposium*, September 30-October 1, 2000, Department of Chemistry, University of Toronto, Canada. (Oral)

8. Prisoners of Alkatraz; A Semi-empirical Study of Encapsulated Small Hydrocarbons in C_{60} Cage, Probing Isotropy of the Internal Space of C_{60} . *University of Isfahan Research Week*, February 26 - March 2, 2000. (Oral)

9. What NMR Can Tell Us About Intermolecular Potential Energy Surfaces. Chemical Physics/Physical Chemistry Seminars, Department of Chemistry, University of Waterloo, Waterloo, Canada, September 29th, 2000. (Oral)

10. Hassan Sabzyan, Anahita Saadatmand, "Observation of the Relaxational Collapse of the Deuteron-Proton J-Coupling Multiplets in the Gas Phase HD Molecule Over a Wide Range of Temperatures and Densities", *Proceedings of The Thirteenth Iranian Chemistry and Chemical Engineering Congress*, February 16-18, 1999, Tarbiat Modarress University, Tehran, I.R. Iran. (Oral)

11. Hassan Sabzyan, "Semi-Empirical Study of 9-Crown-3 and Benzo-9-Crown-3 Gas Phase Complexes with H⁺, Li⁺, Na⁺, Be²⁺ and Mg²⁺ Cations", *Proceedings of The Fifth Iranian Seminar of Inorganic Chemistry*, September 1-2, 1999, University of Isfahan, Isfahan, I. R. Iran. (Oral)

12. Hassan Sabzyan and Mohammad-Bagher Moheb-Ali, A Full Picture for the Pathways of the Pyrolysis Reaction of Methane on the Graphite Surface, *Proceeding of The 7th National Iranian Chemical Engineering Congress (Extended Abstracts)*, Vol. 3, pp. 297-302, University of Teran, (28-31 October, 2002).

13. Hassan Sabzyan and Mohsen Vafaee, " H_2^+ and D_2^+ in intense laser fields", The 3rd SESAME Users Meeting, Sabanci University, Antalya, Turkey, 11-13 October, 2004

14. Hassan Sabzyan, "Ultrashort intense laser fields and their application",(Invited Lecture) 12th Iranian Optics and Photonics Conference, 1-2 February, 2006.

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	اسامی همکاران	عنوان مقاله	گزاری	محل بر ا	عنوان همايش علمي	شمسی	رديف		
			شهر	کشور		دى	ح میلا	تاريږ	
	H. Sabzyan H.	Molecular Dynamics Simulation			International Congress on Nanoscience and Nanotechnology	سال	ماه	روز	
		of Li ₂ C ₂ Nanocrystals	شيراز	ايران		1878	۸	18-70	١
	Nematollahi				ICNN 2010	2010	11	9-11	
	H. Sabzyan S. Gholami				International Congress on	سال	ماه	روز	
		Carbon Nanotorus Maker	شيراز	ايران	Nanoscience and Nanotechnology	١٣٨٩	۸	18-20	۲
					ICNN 2010	2010	11	9-11	
					International Congress on	سال	ماه	روز	
	H. Sabzyan R. Safari	Peltier Coefficient in Molecular Nanoelectronic Systems	شيراز	ايران	Nanoscience and Nanotechnology	1344	۸	۱۸-۲۰	٣
		Tunocecci one Systems			ICNN 2010	2010	11	9-11	
		بكانشا خصيض محمات تقابين			کنفرانس فیزیک ایران ۱۳۸۹ سیزدهمین سمینار شیمیفیزیک ایران	سال	ماه	روز	
	نرگس صادق پور	یت ساختن خروج از عمری برای تمزیع جگالہ الکتامذ	همدان	ايران		١٣٨٩	۶	۲۳-۲۰	۴
		برای وریع پادی ایکترونی				2010	9	11-14	
	H. Sabzyan B. Saed	Efffect of floating basis set			سیزدهمین سمینار شیمیفیزیک ایران ۱۳۸۹	سال	ماه	روز	4
		on the electronic properties	شيراز	ايران		١٣٨٩	١	23-28	۵
		of adamantanes				2010	4	12-15	
	Z. Tavangar H. Sabzyan H. Sabzyan	A computational study of			سیزدهمین سمینار شیمیفیزیک ایران ۱۳۸۹	سال	ماه	روز	
		molecular transport	شيراز	ايران شيرا		١٣٨٩	1	23–28	8
		through carbon hanotubes				2010	4	12-15	
	alstan ano	مطالعه اثر ميدان الكتريج مرجواه	صنعتی ^ن اصفهان		کنفرانس فیزیک ایران ۱۳۸۸	سال	ماه	روز	
	مشل صفري	ده قطعه نانوالکترونیک وملکول پیشنهادی.		ايران		۱۳۸۸	۵	26-28	۷
	رر					2009	8	15-18	
	ای نانوذرات CdSe ی آنها به اندازه حسن سبزیان				115,	سال	ماه	روز	
		مصالعة ويركيهاي فالودرات حسات	اهواز	ايران	تهمین تنفرانس ماده چکال	1848	11	10-18	٨
		و وابستندی الها به الماره				2009	2	4-5	
	حسن سبزیان ریحانه اشرفی	مطالعه نظری و محاسباتی نقاط کوانتومی				سال	ماه	روز	
		مولکولی با هسته بنزنی پرشاخه	كاشان	یران ایران کا	کنفرانس فیزیک ایران	1848	۶	٣-٧	q
		(شششاخهای)			١٣٨٧ 2	2008	8	24-28	

اسامی همکاران	عنوان مقاله	محل برگزاری کشور شهر		جری شمسی خ میلادی معتبر معتبر		جری نا خ میلا	تاريخ ھ تاريز	رديف
M. Vafaee H. Sabzyan	Electron dynamics of H ₂ ⁺ in sub-cycle intense laser pulses	اردبيل	ايران	یازدهمین سمینار شیمیفیزیک ایران ۱۳۸۷	سال ۱۳۸۷ 2008	ماہ 4-5 7	روز ۳۱-۳ 21-24	١٠
Z. Nourisafa H. Sabzyan	Design and quantum computational characterization of molecular quantum dots (دوشاخهای با مجموعه پایه **G++G)	اردبيل	ايران	یازدهمین سمینار شیمیفیزیک ایران ۱۳۸۷	سال ۱۳۸۷ 2008	ماہ 4-5 7	روز ۳۱-۳ 21-24	11
Z. Nourisafa H. Sabzyan	Computational characterization of a family of potential moleculr quantum dots (سەشاخەاى با مجموعە پايە 6-31G)	تهران تربیت مدرس	ايران	The first Conference and Workshop on Mathematical Chemistry ۱۳۸۶	سال ۱۳۸۶ 2008	ماہ ۱۱ 1	روز ۹-۱۱ 29-31	١٢
H. Hamedanian Z. Tavangar A. R. Ashrafi H. Sabzyan	Computing distance matrix and Wiener index of a capped nanotube	تهران تربیت مدرس	ايران	The first Conference and Workshop on Mathematical Chemistry ۱۳۸۶	سال ۱۳۸۶ 2008	ماہ ۱۱ 1	روز ۹–۱۱ 29-31	١٣
S. Hosseini H. Sabzyan	Computational study of the formation of benzyne	تهران تربیت مدرس	ايران	The first Conference and Workshop on Mathematical Chemistry ۱۳۸۶	سال ۱۳۸۶ 2008	ماہ ۱۱ 1	روز ۹–۱۱ 29-31	14
H. Sabzyan M. Vafaee	Rising time effects of ultrashort intense laser field on the enhanced ionization rate of H ₂ ⁺	اصفهان	ايران	دهمین سمینار شیمیفیزیک ایران ۱۳۸۶	سال ۱۳۸۶ 2007	ماد ۲ 4	روز ۳-۶ 23-26	۱۵
F. Taghavi H. Sabzyan	Conformational optical activity in nitrobenzene derivatives	اصفهان	ايران	دهمین سمینار شیمیفیزیک ایران ۱۳۸۶	سال ۱۳۸۶ 2007	ماد ۲ 4	روز ۳-۶ 23-26	18
B. Bouzary H. Sabzyan	NMR lineshapes arising from isolated torsional motion in a complex molecule	اصفهان	ايران	دهمین سمینار شیمیفیزیک ایران ۱۳۸۶	سال ۱۳۸۶ 2007	ماہ ۲ 4	روز ۳-۶ 23-26	۱۷
D. Farmanzadeh H. Sabzyan	Design and theoretical study of a multi-pole molecular switch (مولکولی متفاوت با (۸–۱۶) و (۸–۱۷))	اصفهان	ايران	دهمین سمینار شیمیفیزیک ایران ۱۳۸۶	سال ۱۳۸۶ 2007	ماہ ۲ 4	روز ۳-۶ 23-26	۱۸
Z. Tavangar H. Sabzyan	Simulation of the He-Ar gas mixture flow inside different model 2-D CNT (مخلوط گازها در نانولوله (۱۹،۱۹))	اصفهان	ايران	دهمین سمینار شیمیفیزیک ایران ۱۳۸۶	سال ۱۳۸۶ 2007	ماد ۲ 4	روز ۳-۶ 23-26	١٩

اسامی همکاران	عنوان مقاله	محل برگزاری کشور شهر		عنوان همایش علمی معتبر	تاریخ هجری شمسی تاریخ میلادی		تاريخ ھ تاريعِ	رديف
H. Sabzyan	Correlation between optical activity and topology of electron density for	ر شت	ايران	نهمین سمینار شیم فن یک ایران	سال ۱۳۸۵	ماد ۳	روز ۲۵–۲۲	۲۰
F. Taghavi	small molecules containing two chiral centers			1880	2006	6	13-15	
	Conformational effects			هشتمين سمينار	سال	ماہ	روز	۲۱
H. Sabzyan F. Taghayi	on optical rotation	عهشهد	ايران	شیمیفیزیک ایران	۱۳۸۴	٩	۳-۱	
	(C ₆ H ₅ -CCl ₃ , HOOF, HFN-NFH)			1886	2005	11	21-24	
the transform	مطالعه نظرم ممحاسبات فعالت برنام			سال	ماه	روز		
فريا تقوي	مولکولهای کوچک دارای یک مرکز فعال نوری	خرمآباد	ايران	للفرانس فيريك أيران	1846	۶	٧-١٠	٢٢
	<i>وجوجه</i> و جوړی د د ورو د ورو و د و ورو و ورو و				2005	8	29-31	
E Mahammadi	Structure and electrical	صنعت		هفتمين سمينار	سال	ماه	روز	78 78
H. Sabzyan	conductivity of 1-D and 2-D	اصفهان	ايران	شیمیفیزیک ایران	١٣٨٣	١٢	18-20	
	sourum ratuces			١٣٨٣ :	2005	3	9-11	
S Hosseini	Substituent effects on the		پانزدهمین سمینار شیمی آلی ایران ایران	پانزدهمین سمینار	سال	ماہ	روز	
H. Sabzyan	properties of ortho-benzyne	كرمانشاه		شیمی الی ایران	1846	8	۶-۸	
				17.84	2008	8	28-30	
Z. Nourisafa	of a family of potential			MOLMAT (Molecular Materials) ۱۳۸۷	سال مدينة	ماه	روز ا	۲۵
H. Sabzyan	molecular quantum dots	تولوز	فرانسه		17.44	۴	19-5+	
	(سەشاخەاى با مجموعه پايە **G++G-0-0) Simulation of the He Anges				2008	7	8-11	
Z. Tavangar	mixture flow in model 2-D CNTs			41 st IUPAC World Chemistry Congress ¹ ^π λβ	سال عد ۳۸	ماه	روز ۲۰۰۰ ۲۰۰	18
H. Sabzyan	H. Sabzyan with different (n,m)	نورينو	أيثاليا		2007	ω Q	5 11	
	(مخلوط کارها در نانولولههای (۱۵،۱۵) و (۰،۰۱)) ا : داد ت ف ک تاریخ کا د دداد آندا				2007	0	5-11	
حسن سبزيان	لیررهای یپی فرو توقه و کربردهای آنها (سخنیاز عموم مدعم)	·1 *.	.1.1	لیتیک مفتونس سالا که ارتیک مفتونیک اردان	1876	11	رور ۳۱–۱۱	۲۷
محسن وفايي	ر شعر،تی عبومی مناعو)	سير,ر	'ير'ن	پییات و تو تولیف ،یر،ن ۱۳۸۴	2006	1-2	31-2	
	Simulation of gos flow inside			International Congress on Nanoscience and Nanotechnology ICNN 2006	سال	ماہ	ja,	
Z. Tavangar	different CNT in 2-D models	تهران	ايران		١٣٨۵	٩	77-29	٢٨
H. Sabzyan	(فقط گازهای خالص)				2006	12	18-20	
	Ab initio study of Aflatoxins B and		I	حمار دهمین سمینار	سال	ماه	روز	
N. Alizadeh M. Aghamohammadi	G and their cations, anions and radicals: Predicting structural	ب حند	ادان	پهرونسینی سنیدر شیمی تجزیه ایران ای ۱۳۸۴	۱۳۸۴	۶	۷ – ۹	4
H. Sabzyan	spectroscopic, activity, and chemical properties	بيرجح	0.7.		2005	8	29-31	

اسامی همکاران	عنوان مقاله	محل برگزاری کشور شهر		محل برگزاری عنوان همایش علمی معتبر کشور شهر		تاریخ هجری شمسی تاریخ میلادی		
M. Mokhtari H. Sabzyan M. R. Noorbala	Intramolecular oxygen exchange in some heterocyclic compounds	صنعتی اصفهان	ايران	هفتمین سمینار شیمیفیزیک ایران ۱۳۸۳	سال ۱۳۸۳ 2005	ماہ ۱۲ 3	روز ۱۸-۲۰ 9-11	٣٠
R. Amiri H. Sabzyan M. Tafazzoli	Ionic strength effect on the NMR spectrum of simple organic solutes	صنعتی اصفهان	ايران	هفتمین سمینار شیمیفیزیک ایران ۱۳۸۳	سال ۱۳۸۳ 2005	ماہ ۱۲ 3	روز ۱۸-۲۰ 9-11	۳۱
M. Vafaee H. Sabzyan	Calculation of the ionization rate of H_2^+ in intense laser fields	صنعتی اصفهان	ايران	هفتمین سمینار شیمیفیزیک ایران ۱۳۸۳	سال ۱۳۸۳ 2005	ماہ ۱۲ 3	روز ۱۸-۲۰ 9-11	٣٢
B. Buzari H. Sabzyan	Effect of vibrational motion on the magnetic shielding	صنعتی اصفهان	ايران	هفتمین سمینار شیمیفیزیک ایران ۱۳۸۳	سال ۱۳۸۳ 2005	ماہ ۱۲ 3	روز ۱۸-۲۰ 9-11	٣٣
H. Sabzyan H. Ebadi	Ionization of a 1-D model of H_2^+ in different states in intense laser fields	مشهد	ايران	هشتمین سمینار شیمیفیزیک ایران ۱۳۸۴	سال ۱۳۸۴ 2005	ماہ ۹ 11	روز ۳-۱ 21-24	٣۴
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