Curriculum Vitae

A Brief Description

Nasser L. Hadipour

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Address: Physical Chemistry Department, Faculty of Sciences, Tarbiat Modares University, Tehran, Iran. P.O.Box 14115-175

Academic Rank

Full Professor of Physical Chemistry, Tarbiat Modares University, Tehran, Iran.

Education

Sabbatical

Visiting fellow at Institute of Chemistry, Academia Sinica of Taiwan (Sept. 2007- Sept. 2008)

Postdoctoral fellowship

University of New York, New York, USA, 1985-1986.

PhD

Physical Chemistry, University of Massachusetts Amherst, Massachusetts, USA, 1985.

MSC

Physics, University of Massachusetts Amherst, Massachusetts, USA,1983.

Chemistry, Northeastern University, Massachusetts, USA,1981.

BSC

Chemistry, Sharif University of Technology, Tehran, Iran. 1976.

Language Skills

1. **Persian**

Speaking: Native, Reading: Native, Writing: Native

2. **English-close to native**

Speaking: Native, Reading: Native, Writing: Native

Teaching Experience

A) Taught Undergraduate Courses

General Chemistry I & II

Physical Chemistry I & II

Elementary Quantum Chemistry

Basic Molecular Spectroscopy

B) Taught Graduate Courses

Advanced Physical Chemistry

Modern Quantum Chemistry

Statistical Thermodynamics I & II

Advanced Molecular Spectroscopy

NMR Spectroscopy

Research Interests

Density Functional Theory (DFT) calculations

Molecular dynamics simulations of biological systems and nanostructures

Investigation of hydrogen bonds in crystalline phase using ab initio calculations

List of Publications

[112] Density functional theory evaluation of pristine and BN-doped biphenylene nanosheets to detect HCN R Esfandiarpour, MR Hosseini, NL Hadipour, A Bahrami. Journal of Molecular Modeling 2019, 25 (6), 163.

[111] Influence of dendrimer surface chemistry and pH on the binding and release pattern of chalcone studied by molecular dynamics simulations. F Badalkhani-Khamseh, A Ebrahim-Habibi, NL Hadipour.Journal of Molecular Recognition 2019, 32 (1), e2757.

[110] The influence of the structural variations of the fused electron rich-electron deficient unit in the π-spacer of A-D-π-D-A organic dyes on the efficiency of dye-sensitized solar cells: A computational study. E Hosseinzadeh, NL Hadipour. Organic Electronics 2018, 62, 43-55.

[109] Bare surface of gold nanoparticle induces inflammation through unfolding of plasma fibrinogen. B Kharazian, SE Lohse, F Ghasemi, M Raoufi, AA Saei, F Hashemi, et al. Scientific Reports 2018, 8 (1), 12557.

[108] Atomistic computer simulations on multi-loaded PAMAM dendrimers: a comparison of amine-and hydroxyl-terminated dendrimers. F Badalkhani-Khamseh, A Ebrahim-Habibi, NL Hadipour. Journal of computer-aided molecular design 2017, 31 (12), 1097-1111.

[107] Molecular engineering of bithiazole-based organic dyes with different electron-rich linkers toward highly efficient dye-sensitized solar cells. E Hosseinzadeh, NL Hadipour, G Parsafar. Journal of Photochemistry and Photobiology A: Chemistry 2017, 349, 171-182.

[106] DFT, QTAIM, and NBO studies on the trimeric interactions in the protrusion domain of a piscine betanodavirus. EK Astani, NC Chen, YC Huang, A Bahrami, LY Chen, PR Lin, HH Guan, et al. Journal of Molecular Graphics and Modelling 2017, 78, 61-73.

[105] A theoretical study on quadrupole coupling parameters of HRPII Protein modeled as 310-helix & α-helix structures. F Elmi, N Hadipour. Quarterly Iranian Chemical Communication 2017, 5, 372-380.

[104] Complexation of nicotinic acid with first generation poly (amidoamine) dendrimers: A microscopic view from density functional theory. F Badalkhani-Khamseh, A Bahrami, A Ebrahim-Habibi, NL Hadipour. Chemical Physics Letters 2017, 684, 103-112.

[103] The electronic and structural responses of B12N12 nanocage toward the adsorption of some nonpolar X2 molecules: X=(Li, Be, B, N, O, F, Cl, Br, I): A DFT approach. A Bahrami, MB Qarai, NL Hadipour. Computational and Theoretical Chemistry 2017, 1108, 63-69.

[102] Molecular interactions investigated with DFT calculations of QTAIM and NBO analyses: An application to dimeric structures of rice α-amylase/subtilisin inhibitor. EK Astani, NL Hadipour, CJ Chen. Chemical Physics Letters 2017, 672, 80-88.

[101] A computational investigation on the influence of different π spacer groups in the bithiazole-based organic dye sensitizers on the short-circuit photocurrent densities of dye-sensitized solar cells. E Hosseinzadeh, NL Hadipour, G Parsafar. Journal of Photochemistry and Photobiology A: Chemistry 2017, 333, 70-78.

[100] A DFT study on the functionalization of C60 fullerene with 1, 2-benzoquinone. MK Hazrati, NL Hadipour. Computational and Theoretical Chemistry 2016, 1098, 63-69.

[99] DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. M Mirzaei, O Gülseren, N Hadipour. Computational and Theoretical Chemistry 2016, 1090, 67-73.

[98] A theoretical study on the characteristics of the intermolecular interactions in the active site of human androsterone sulphotransferase: DFT calculations of NQR and NMR parameters and QTAIM analysis. EK Astani, E Heshmati, CJ Chen, NL Hadipour. Journal of Molecular Graphics and Modelling 2016, 68, 14-22.

[97] Relaxations of fluorouracil tautomers by decorations of fullerene-like SiCs: DFT studies. A Kouchaki, O Gülseren, N Hadipour, M Mirzaei. Physics Letters A 2016, 380 (25-26), 2160-2166.

[96] A study of hydrogen bond effects on the oxygen, nitrogen, and hydrogen electric field gradient tensors in the active site of human dehydroepiandrosterone sulphotransferase: A density functional theory based treatment. E Astani, E Heshmati, CJ Chen, NL Hadipour, S Shekarsaraei. Chemical Physics Letters 2016, 653, 78-84.

[95] Understanding the nanoparticle–protein corona complexes using computational and experimental methods. B Kharazian, NL Hadipour, MR Ejtehadi. The international journal of biochemistry & cell biology 2016, 75, 162-174.

[94] DFT studies of NH---Cl hydrogen bond of amino acid hydrochloride salts in ion channels. M Moridi, S Shekarsaraei, NL Hadipour. Acta Chimica Slovenica 2016, 63 (2), 241-250.

[93] Noncovalent intermolecular interactions between dehydroepiandrosterone and the active site of human dehydroepiandrosterone sulphotransferase: A density functional theory based treatment. E Astani, E Heshmati, CJ Chen, NL Hadipour, S Shekarsaraei. Chemical Physics Letters 2016, 649, 123-129.

[92] Adsorption behavior of 5-fluorouracil on pristine, B-, Si-, and Al-doped C60 fullerenes: A first-principles study. MK Hazrati, NL Hadipour. Physics Letters A 2016, 380 (7-8), 937-941.

[91] Interplay between Tetrel and Triel Bonds in RC6H4CN center dot center dot center dot MF3CN center dot center dot center dot BX3 Complexes: A Combined Symmetry-Adapted …. S Yourdkhani, T Korona, NL Hadipour. Journal Of Computational Chemistry 2015, 36 (32), 2412-2428.

[90] Interplay between tetrel and triel bonds in RC6H4CN··· MF3CN··· BX3 complexes: A combined symmetry-adapted perturbation theory, Møller-Plesset, and quantum theory of atoms-in …. S Yourdkhani, T Korona, NL Hadipour. Journal of computational chemistry 2015, 36 (32), 2412-2428.

[89] A Computational Study of N–H… O Hydrogen Bonding to Investigate Cooperative Effects. S Shekarsaraei, M Moridi, NL Hadipour. World Academy of Science, Engineering and Technology, International Journal of Chemical and Molecular Engineering 2015, 9 (3).

[88] Structure and Energetics of Complexes of B12N12 with Hydrogen Halides: SAPT(DFT) and MP2 Study. S Yourdkhani, T Korona, NL Hadipour. The Journal of Physical Chemistry A 2015, 119 (24), 6446-6467.

[87] Theoretical study on the Al-doped ZnO nanoclusters for CO chemical sensors. NL Hadipour, A Ahmadi Peyghan, H Soleymanabadi. The Journal of Physical Chemistry C 2015, 119 (11), 6398-6404.

[86] Theoretical investigation on the selective detection of SO2 molecule by AlN nanosheets. SF Rastegar, NL Hadipour, H Soleymanabadi. Journal of molecular modeling 2014, 20 (9), 2439.

[85] DFT study of NH3 adsorption on pristine, Ni-and Si-doped graphynes. AA Peyghan, SF Rastegar, NL Hadipour. Physics Letters A 2014, 378 (30-31), 2184-2190.

[84] Theoretical investigation of azo dyes adsorbed on cellulose fibers: 2. Spectroscopic study. F Zanjanchi, NL Hadipour, H Sabzyan, J Beheshtian. Journal of the Iranian Chemical Society 2014, 11 (1), 111-121.

[83] A DFT study on doping assisted changing of B80 electronic structure: Promising candidates for NH3 sensor. A Bahrami, S Yourdkhani, MD Esrafili, NL Hadipour. Sensors and Actuators B: Chemical 2014, 191, 457-463.

[82] Density functional theory studies of carbon nanotube—graphene nanoribbon hybrids. A Omidvar, NL Hadipour. Journal of the Iranian Chemical Society 2013, 10 (6), 1239-1246.

[81] Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures. F Zanjanchi, NL Hadipour, H Sabzyan, J Beheshtian. Journal of the Iranian Chemical Society 2013, 10 (5), 985-999.

[80] DFT studies of acrolein molecule adsorption on pristine and Al-doped graphenes. SF Rastegar, NL Hadipour, MB Tabar, H Soleymanabadi. Journal of molecular modeling 2013, 19 (9), 3733-3740.

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[77] NO2 detection by nanosized AlN sheet in the presence of NH3: DFT studies. SF Rastegar, AA Peyghan, HR Ghenaatian, NL Hadipour. Applied Surface Science 2013, 274, 217-220.

[76] A computational investigation of the electronic properties of Octahedral AlnNn and AlnPn cages (n = 12, 16, 28, 36, and 48). M Saeedi, M Anafcheh, R Ghafouri, NL Hadipour. Structural Chemistry 2013, 24 (2), 681-689.

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Solar Energy Materials and Solar Cells 2012, 105, 125-131.

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[68] The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. A Ahmadi, M Kamfiroozi, J Beheshtian, NL Hadipour. Structural Chemistry 2011, 22 (6), 1261.

[67] A computational NICS and 13C NMR characterization of BN-substituted 60C fullerenes. M Anafcheh, NL Hadipour. Physica E: Low-dimensional Systems and Nanostructures 2011, 44 (2), 400-404.

[66] Characteristics and nature of halogen bonds in linear clusters of NCX (X= Cl, and Br): an ab initio, NBO and QTAIM study. MD Esrafili, NL Hadipour. Molecular Physics 2011, 109 (20), 2451-2460.

[65] Computational study on the characteristics of the interaction in linear urea clusters. MD Esrafili, J Beheshtian, NL Hadipour. International Journal of Quantum Chemistry 2011, 111 (12), 3184-3195

[64] Interaction of NH3 with aluminum nitride nanotube: electrostatic vs. covalent. A Ahmadi, J Beheshtian, NL Hadipour. Physica E: Low-dimensional Systems and Nanostructures 2011, 43 (9), 1717-1719.

[63] Investigating purine-functionalised carbon nanotubes and their properties: a computational approach. M Mirzaei, HR Kalhor, NL Hadipour. IET nanobiotechnology 2011, 5 (2), 32-35.

[62] Study of CO··· HN Hydrogen bond interactions in amyloid beta (Aβ): A DFT study of the electric field gradient and CS tensors and NBO analysis. H Behzadi, NL Hadipour, M Mousavi-khoshdel. Computational and Theoretical Chemistry 2011, 965 (1), 137-145.

[61] Photo-oxidation of phenylazonaphthol dyes and their reactivity analysis in the gas phase and adsorbed on cellulose fibers states using DFT and TD-DFT. F Zanjanchi, NL Hadipour, H Sabzyan, J Beheshtian. Dyes and Pigments 2011, 89 (1), 16-22.

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[59] DFT study of CH4 adsorption on the (5,0), (4,4), (5,5) and (6,6) single-walled carbon nanotubes. Calculated binding energies, NMR and NQR parameters. BB Shirvani, MB Shirvani, J Beheshtian, NL Hadipour. Journal of the Iranian Chemical Society 2011, 8 (1), S110-S118.

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[54] DFT study of NH3 adsorption on the (5, 0), (8, 0), (5, 5) and (6, 6) single-walled carbon nanotubes. Calculated binding energies, NMR and NQR parameters. BB Shirvani, J Beheshtian, MD Esrafili, NL Hadipour. Physica B: Condensed Matter 2010, 405 (6), 1455-1460.

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[52] Ab Initio Calculations of 14n NQR Parameters and 13C, 1H, And 15N Chemical Shifts Including A Comparison with Experimental NMR Data for Cyclotrisazobenzene. N Zamand, AR Aliakbar, NL Hadipour. Journal of Theoretical and Computational Chemistry 2009, 8 (04), 647-656.

[51] Density functional theory study of atomic oxygen, O2 and O3 adsorptions on the H-capped (5, 0) single-

walled carbon nanotube. R Khorrampour, MD Esrafili, NL Hadipour. Physica E: Low-dimensional Systems and Nanostructures 2009, 41 (8), 1373-1378.

[50] A density functional study of 15N chemical shielding tensors in quinolines. H Behzadi, MD Esrafili, J Beheshtian, NL Hadipour, D van der Spoel. Chemical Physics Letters 2009, 476 (4-6), 196-200.

[49] Characterization of cooperative effects in linear α-glycylglycine clusters. A Bahrami, MD Esrafili, NL Hadipour. Biophysical chemistry 2009, 143 (1-2), 26-33.

[48] Study of hydrogen bonds in crystalline 5-nitrouracil. Density functional theory calculations of the O-17, N-14, and H-2 nuclear quadrupole resonance parameters. M Mirzaei, NL Hadipour. Journal of the Iranian Chemical Society 2009, 6 (1), 195-199.

[47] Structure and electronic properties of hydrogen chemisorption on boron nitride nanotubes. J Beheshtian, H Behzadi, Z Bagheri, NL Hadipour 2009.

[46] 15N Chemical Shift Calculations and Natural Bonding Orbital Analyses of (Benzamide) N= 1-6 Clusters. MD Esrafili, J Beheshtian, NL Hadipour. Journal of Theoretical and Computational Chemistry 2009, 8 (supp01), 973-982.

[45] Electronic structure characterization of FeIII-protoporphyrin IX (FeIII-PPIX) and β-hematin using calculated nuclear quadrupole resonance (NQR) and Mössbauer parameters. MA Rafiee, NL Hadipour. Canadian Journal of Chemistry 2008, 86 (12), 1095-1098.

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[41] Theoretical study of N–H··· O hydrogen bonding properties and cooperativity effects in linear acetamide

clusters. MD Esrafili, H Behzadi, NL Hadipour. Theoretical Chemistry Accounts 2008, 121 (3-4), 135-146

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SA Khorami. Journal of Molecular Graphics and Modelling 2018, 26 (6), 977-981.

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[18] Structural Elucidation of {[(CH3)2SnCl2·H2O]2·18-crown-6} n and its Hydrogen Bonding in Solution by HMBC Spectroscopy. MM Amini, A Azadmher, HR Bijanzadeh, N Hadipour. Journal of inclusion phenomena and macrocyclic chemistry 2006, 54 (1-2), 77-80.

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nuclear quadrupole coupling constants. NL Hadipour, F Elmi. Chemical physics letters 2003, 371 (1-2), 56-61.

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