

Curriculum Vitae



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Present Occupation Associate Prof.

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Educational Qualification

| Degree | University | Year |
|-------------------------------|---------------------------------------|------|
| B.Sc. (Pure Chemistry) | Isfahan University (Isfahan, Iran) | ۱۹۹۰ |
| M.Sc. (Physical Chemistry) | Isfahan University (Isfahan, Iran) | ۱۹۹۳ |
| Ph.D. (Quantum Chemistry) | Shiraz University (Shiraz, Iran) | ۱۹۹۸ |

Teaching Experience (۱۹۹۹-۲۰۱۲)

Taught the following graduate and undergraduate courses:

General Chemistry, Physical Chemistry, Physical Chemistry Lab., Advanced Physical Chemistry, Quantum Chemistry, Molecular Spectroscopy, Organic Physical Chemistry, Computer Programming, Mathematical Methods in Physical Chemistry.

Research Experience

Quantum Calculations, Explosives, Propellants.

The Title of the MSC Dissertation (۱۹۹۳)

The Investigation of the High Pressures on the Displacement of the Radial Distribution of The Hydrogen Atom in Ground State

The Title of the PhD Dissertation (۱۹۹۸)

First and Second Analytical Derivatives of Molecular Integrals for Calculations of Energy Using Spherical Gaussian & Application of Simplified PV-RR Procedure for H_v and LiH Molecules & Lone Pair Description in FSGO Method for Some Cyclic Carbenes.

List of the Publications (۱۹۹۷-۲۰۱۱)

۱. A. H. Pakyari and **M. Oftadeh**, "First Derivative of Molecular Integrals for Electronic Energy Using Spherical Gaussian Type Orbitals", *J. Molecular Structure (THEOCHEM)*, ۳۸۹, (۱۹۹۷).
۲. A. H. Pakyari and **M. Oftadeh**, "Analytical Second Derivatives of Molecular Integrals Obtained by Spherical Gaussian Orbital", *J. Molecular Structure (THEOCHEM)*, ۴۳۰, (۱۹۹۸).
۳. M. H. Keshavarz and **M. Oftadeh**, "A New Correlation for Predicting the C-J Pressure of CHNO Explosive", *High Temperature-High Pressure*, ۳۴, ۴۹۰ (۲۰۰۲).
۴. M. H. Keshavarz and **M. Oftadeh**, "Two New Correlations for Predicting Detonation Power of CHNO Explosives", *Bull. Korean Chem. Soc.*, ۲۴(۱), ۱۹ (۲۰۰۳).
۵. M. H. Keshavarz and **M. Oftadeh**, "New Estimated Method for Heat of Formation of CHNO Explosives in Solid State", *High Temperature-High Pressure*, ۴۶ (۲۰۰۴).
۶. M. H. Keshavarz and **M. Oftadeh**, "Simple Method of Predicting Detonation Pressure of CHNO Mixed Explosives", *Indian J. Eng. Mater. Sci.*, ۱۰ (۲۰۰۳)
۷. M. H. Keshavarz and **M. Oftadeh**, "Performance Study of Energetic Compound ۲,۴,۶-Trinitro-۱,۳,۵-Triazine", *Asian J. Chem.*, ۱۷(۲) (۲۰۰۵)
۸. M. H. Keshavarz and **M. Oftadeh**, "Performance Study of ۱,۱-Dimethyl-۲-Cyanoethylhydrazine as Liquid Propellant", *Theory and Practice of Energetic Materials*, ۵ (۲۰۰۳).
۹. M. H. Keshavarz and **M. Oftadeh**, "New Method for Predicting of C-J Detonation Velocity of CHNO Explosives at Any Loading Density", *Theory and Practice of Energetic Materials*, ۵ (۲۰۰۳).
۱۰. M. Salavati Niasari, S. Abdolmohammadi and **M. Oftadeh**, "Host (Nanopores of Zeolite-Y)/Guest (Co(II)-Azamacrocyclic Complexes) Nanocomposite Materials: Synthesis,

Characterization and Catalytic Epoxidation of Styrene with Molecular Oxygen”, *J. Coord. Chem.*, ۶۱(۱۷), ۲۸۳۷, ۲۰۰۸.

۱۱. A. Semnani, H. R. Pouretedal, M. F. keshavarz, A. R. Firooz and **M. Oftadeh**, “Interaction Between ۱, ۳, ۵-Trithiane and Iodine Monobromide in Halomethane Solutions”, *Heterocyclic Commu.*, ۱۴(۳), ۲۰۶, ۲۰۰۸.
۱۲. **M. Oftadeh**, M. Salavati Niasari and F. Davar, “Synthesis of ZnO Nanoparticles and Their Optical Properties”, *Int. J. Nanoparticles*, ۲, ۳۰۷, ۲۰۰۹.
۱۳. **M. Oftadeh**, M. Salavati Niasari and F. Davar, “Sized-Controlled ZnO Nanoparticles, Synthesis and Morphology”, *Int. J. Nanoscience*, ۳, ۲۷۷, ۲۰۰۹.
۱۴. A. Semnani, A.R. Firooz, H.R. Pouretdal, M.H. Keshavarz and **M. Oftadeh**, “Complex Formation Between Some Thiocrownethers and ۱,۳,۵-Trithian with Bromine in Gas Phase and Carbon Tetrachloride Solution”, *Chemistry*, ۱۹, ۸۰, ۲۰۱۰.
۱۵. **Mohsen Oftadeh**, Masoud Hamadiani Khozani, Mahshid Radhoosh, Mohammad Hossein Keshavarz, DFT molecular orbital calculations of initial step in decomposition pathways of TNAZ and some of its derivatives with –F, –CN and –OCH₃ groups, *Computational and Theoretical Chemistry* ۹۶۴ (۲۰۱۱) ۲۶۲–۲۶۸.
۱۶. **M. Oftadeh**, S. Naseh, M. Hamadiani, Electronic properties and dipole polarizability of thiophene and thiophenol derivatives via density functional theory, *Computational and Theoretical Chemistry* ۹۶۶ (۲۰۱۱) ۲۰-۲۵.
۱۷. **Mohsen Oftadeh**, Nafice Makkei, Mahnaz Khosravi Farsani, Investigation of adsorption process and thermodynamics of cochineal dye on wool, *Journal of Materials Science and Engineering B, USA*, ۱ (۲۰۱۱) ۳۸۸-۳۹۳.
۱۸. **M. Oftadeh**, A. Aghtar, M. Nasr Esfahani, Masoud Salavati-Niasari, N. Mir, Fabrication of highly efficient dye-sensitized solar cell and CO₂ reduction photocatalyst using TiO₂ nanoparticles prepared by spin coating assisted sol-gel method, *Journal of Iranian Chemical Society*, xx (۲۰۱۱) xxx-xxxx. In Press.
۱۹. **Mohsen Oftadeh**, Leila Tavakolizadeh, Investigation of optoelectronic properties of N₃ dye-sensitized TiO₂ nanocrystals by hybrid methods: ONIOM (QM/MM) calculations, *International Nano Letters*, ۲(۱) (۲۰۱۱) ۵-۹.
۲۰. Nosrat Madadi Mahani, **Mohsen Oftadeh**, Kinetic and thermodynamic study of activated Carbon from pistachio shell by thermogravimetric method, *Journal of Materials Science and Engineering A, USA*, ۱ (۲۰۱۱) ۸۸۷-۸۹۱.

Conference Papers (۲۰۰۱- ۲۰۱۱)

۱. M. H. Keshavarz and **M. Oftadeh**, “Performance of ۲, ۴-Dinitroimidazole as a Insensitive Energetic Material”, ۲nd International Pyrotechnics Seminar, Australia, ۴۲۱-۴۲۳ (۲۰۰۱).
۲. M. H. Keshavarz and **M. Oftadeh**, “A New Correlation for Predicting Detonation Properties of Explosives”, ۲nd International Pyrotechnics Seminar, Australia, ۴۱۷-۴۲۰ (۲۰۰۱).
۳. M. H. Keshavarz and **M. Oftadeh**, “Detonation Properties of ۲, ۴, ۶-Trinitro-۱,۳,۵-Triazine (TNTA) as a High-Energy Density Explosive”, ۴th Physical Chemistry Seminar, Booshehr, Iran, March ۲۰۰۱.
۴. M. H. Keshavarz and **M. Oftadeh**, “Behavior of Hydroxyethylhydrazine as Liquid Propellant and Composition Detonation Products of ۲۴-DNI with BKW-EOS”, ۵th Physical Chemistry Seminar, Tehran, Iran, Feb., ۲۰۰۲.
۵. M. H. Keshavarz and **M. Oftadeh**, “Study of Performance of ۲۴-DNI as a Solid Oxidizer in Rocket Propellant”, ۵th Physical Chemistry Seminar, Tehran, Iran, Feb., ۲۰۰۲.
۶. **M. Oftadeh** and M. H. Keshavarz, “The Synthesis of Fullerene C_{۶۰} by Simple Arc Method”, ۵th Physical Chemistry Seminar, Tehran, Iran, Feb., ۲۰۰۲.
۷. M. H. Keshavarz and **M. Oftadeh**, “Study of P_{cj} Correlation Aided by PM^۳ Procedure for Condensed CHNO Explosives”, ۳rd ASPEP Conference, France ۲۰۰۳.
۸. M. H. Keshavarz and **M. Oftadeh**, “Study of the Performance of ۱-Methyl-۱-cyanoethylhydrazine as a Liquid Mono- and Bipropellant”, ۳rd ASPEP Conference, France ۲۰۰۳.
۹. M. H. Keshavarz and **M. Oftadeh** “Performance Study of ۱,۱-dimethyl-۲-cyanoethylhydrazine as Liquid Propellant”, ۸th AISPEP Conference, China, ۲۰۰۳.
۱۰. M. H. Keshavarz and **M. Oftadeh**, “New Method for Predicting od CJ Detonation Velocity of CHNO Explosives at any Loading Density” , ۸th AISPEP Conference, China, ۲۰۰۳.
۱۱. M. H. Keshavarz and **M. Oftadeh**, “Theoretical Study of K-۶ as High Performance Explosive and Oxidizer”, ۸th AISPEP Conference, China, ۲۰۰۳.
۱۲. M. Oftadeh, “The Investigation of the propellant performance of Some of the Nitroguanidine, Azol Derivatives and Nitroamides Compounds as Gas Generators”, ۱۱th Asian Chemical Congress, Korea, ۲۰۰۵.
۱۳. M. Hamadianian and **M. Ofatdeh**, “Investigation of Explosive Performance of mono-, Bi- and Tri-cyclic Nitramines by ab-initio Computational Methods”, MCC ۲۰۰۶ , Croatia, ۲۰۰۶.

۱۴. **M. Oftadeh** and M. Hamadianian, “The Investigation of the Deflagration Pathway of CHNOF Explosives of Mono and Di Cyclic nitramine Compounds by Ab initio and semiempirical calculations”, ۴۱st IUPAC World Chemistry Congress, Turin, Italy, Aug. ۲۰۰۷.
۱۵. M. Hamadianian and **M. Oftadeh**, “The Investigation of the Deflagration Pathway of CHNOF Explosives of tri-Cyclic Nitramine Compounds by Ab Initio and Semiempirical Calculations”, ۴۱st IUPAC World Chemistry Congress, Turin, Italy, Aug. ۲۰۰۷.
۱۶. **M. Oftadeh** and M. Salavati niasari, “Synthesis, Characterization and Catalytic Oxidation by Host (Nanocage of Zeolite-Y)/Guest (Metal Complexes of ۱۲-Membered Thio Macroyclic Schiff-base Ligand) Nano Composite Materials”, IXth Netherlands' Catalysis and Chemistry Conference, Noordwijkerhout, Netherlands, March ۲۰۰۸.
۱۷. **M. Oftadeh**, N. Makkei and M. Khosravi Farsani, “An Adsorption and Thermodynamic Study of Cochineal Dyeing on Wool”, PACCON۲۰۰۹, Phistanulok, Thailand, Jan. ۲۰۰۹.
۱۸. **M. Oftadeh**, M Salavati Niasari and F. Davar, “Nanodimensional microreactors encapsulation of ۱۵- and ۱۶-membered macrocyclic Schiff-base copper(II) complex nanoparticles: catalytic oxidation”, XIth Netherlands Catalysis and Chemistry Conference, Netherlands, March ۲۰۱۰.
۱۹. **M. Oftadeh** and M. Moghadari, “ Donor-acceptor in the charge transfer molecular complexes of C₆S₄H₈ and C₇S₅H_{1۲} with dihalogenes: DFT method”, Fourth Humboldt Conference on Computational Chemistry, Bulgaria, July ۲۰۱۰.
۲۰. **M. Oftadeh** and L. Tavakolizadeh, “Investigation of optical properties of sensitized TiO₂ nanoparticles by N₂ with ONIOM method”, ۳rd International Congress on Nanoscience and Nanotechnology (ICNN۲۰۱۰), Shiraz, Iran, Nov ۲۰۱۰.

Recent Research Projects Completed (۲۰۰۰- ۲۰۱۱)

۱. **M. Oftadeh** and M. H. Keshavarz, “Synthesis and Evaluation of The Explosive and Propellant Performance of High Energetic ۲,۴-dimethylimidazol”, Malek Ashtar University, Shahinshar, Isfahan (۲۰۰۰).
۲. M. H. Keshavarz and **M. Oftadeh**, “Synthesis and Evaluation of Many Low Volatile Hydrazine Derivatives for Using in Missiles with Liquid Fuels”, Malek Ashtar University, Shahinshar, Isfahan (۲۰۰۰).
۳. **M. Oftadeh** and M. K. Keshavarz, “Investigation of Explosive Performance of Dense Fluid by Using Equation of State”, Payame Noor University, Isfahan (۲۰۰۴).

۴. **M. Oftadeh** and M. Hashmi Talkhoncheh, “Laboratory Synthesis of Diallylester” Isfahan Payame Noor University, Isfahan (۲۰۰۵).
۵. **M. Oftadeh** and M. Hamadian, “Investigation of The Degradation Pathways for Many Mono, Di and Tri Cyclic Compounds of CHNOF Explosives by Ab Initio and Semiepermerical Methods”, Payame Noor University, Isfahan (۲۰۰۷).
۶. **M. Ofatdeh** and M. Salavati Niasari, “Host/Guest Nanocomposite Materials (HGNM): Synthesis, Characterization and Catalytic Activity”, Payame Noor University, Isfahan (۲۰۱۰).
۷. **M. Ofatdeh**, “AM¹ Study of Acidities of Fulleropyrrolindines in Gas and Solution Phases”, Payame Noor University, Isfahan (۲۰۱۰).
۸. **M. Oftadeh**, “Theoretical Study and Investigation of the Adsorption of N⁺ Dye and Its Derivatives on the TiO₂ Nanoparticles as an Electrode using in DSSC by DFT Method”, Payame Noor University, Isfahan (۲۰۱۱).

Recent Books

- ۱- **M. Oftadeh** and M. Hamadian, “*General Chemistry in Laboratory*”, Samaghalam Publications (۲۰۰۶).
- ۲- **M. Oftadeh**, “*English for Chemistry Students*”, Payame Noor University Publications (۲۰۰۶)
- ۳- **M. Oftadeh**, “Physical Chemistry I”, translated of “Physical Chemistry” by R. G. Mortimer, ۳rd edition, Elsevier publications, in Persian (۲۰۱۰).

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