

## IN THE NAME OF GOD

### Curriculum Vitae

*Dr. Adel Reisi-Vanani*

Assistant Professor of Physical Chemistry

Corresponding Address:

Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, P.O. Box. 87317-51167, Kashan, I.R. Iran

**E-mail:** *areisi@kashanu.ac.ir*

**Tel:** (++98)31-55912358

**Fax:** (++98)31-55912397

### Research Activity

Nanoparticles

Nanocatalyst

Theoretical investigation of nanostructures

Theoretical study of the kinetic and Thermodynamic properties of reactions

Quantum calculations

Hydrogen storage

Adsorption

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.)

#### Journal Publications:

1. **Adel Reisi-Vanani**, Ali Asghar Rezaei, Evaluation of the aromaticity of non-planar and bowl-shaped molecules by NICS criterion, *J. Mol. Graph. Model.* (2015) Accepted.
2. **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, *J. of Nanostructures* 4 (2014) 153-159.
3. M. Izadyara, N. Zavar, M.R. Housaindokht, M. Khavani, **A. Reisi-Vanani**, Secondary Structure Effects on the Acidity of Histidine and Lysine-Based Peptides Model; A Theoretical Study, *Phys. Chem. Res.*, 3(1) (2015) 67-77.
4. **Adel Reisi-Vanani** , Leila Shahrokh, Syamak Nasiri Kokhdan, Theoretical study of the corannulene ozonolysis and evaluation of the various reaction paths, *Computational and Theoretical Chemistry*, 1051 (2015) 72–78, DOI: [10.1016/j.comptc.2014.11.002](https://doi.org/10.1016/j.comptc.2014.11.002)
5. **A. Reisi-Vanani**, S. Faghih, 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*, (2015) DOI: 10.1080/10406638.2014.948966

6. **A. Reisi-Vanani**, S. Hoseinpour, A computational study of the mechanism and kinetics for gas-phase decomposition and reactivity of the  $C_4F_9OCH_2O$  radical between 200 and 400 K, *Prog. React. Kinet. Mech.* 40(1) (2015) 59-68.
7. **A. Reisi-Vanani**, S. Hoseinpour, A theoretical investigation of decomposition and reactivity of the atmospheric  $C_3F_7OCH_2O$  radical, *Arabian Journal of Chemistry*, 2013, <http://dx.doi.org/10.1016/j.arabjc.2013.05.030>.
8. **A. Reisi-Vanani**, Leila 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.
9. **A. Reisi-Vanani**, Soudeh 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. <http://dx.doi.org/10.1016/j.jscs.2014.02.003>.
10. **A. Reisi-Vanani**, M. Izadyar, A Theoretical Study on the Mechanism and Kinetic of the Thermal Decompose of Carbamoyl Azide, *Prog. React. Kinet. Mech.* 38(3) (2013) 305 – 315.
11. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, V. Jabbari, Photodeposition-Assisted Synthesis of Novel Nanoparticulate In, S-codoped  $TiO_2$  Powders with High Visible Light-Driven Photocatalytic Activity, *Appl. Surf. Sci.* 285 (2013) 121–129. <http://dx.doi.org/doi:10.1016/j.apsusc.2013.07.165>.
12. M. Hamadani, **A. Reisi-Vanani**, M. Behpour, A.S. Esmaily, Synthesis and characterization of Fe,S-codoped  $TiO_2$  nanoparticles: Application in degradation of organic water pollutants, *Desalination*, 281 (2011) 319–324.
13. M. Hamadani, **A. Reisi-Vanani**, A. Majedi, Synthesis, characterization and effect of calcination temperature on phase transformation and photocatalytic activity of Cu,S-codoped  $TiO_2$  nanoparticles, *Appl. Surf. Sci.* 256 (2010) 1837-1844.
14. M. Hamadani, **A. Reisi-Vanani** and A. Majedi, Sol-Gel Preparation and Characterization of Co/ $TiO_2$  Nanoparticles: Application to the Degradation of Methyl Orange, *J. Iran. Chem. Soc.*, 7 (2010) S52-S58.

15. 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, *Mater. Chem. Phys.* 116 (2009) 376–382.

**Conference papers:**

1. Somayeh 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**.
2. Soudeh 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**.
3. Leila 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**.
4. Leila 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**.
5. Sajedin Hoseinpour, **Adel Reisi-Vanani**, Maryam Shamshiri, 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**.
6. 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**.
7. **Adel Reisi-Vanani**, S. Hoseinpour, Theoretical studies of decomposition and reactivity of the C<sub>3</sub>F<sub>7</sub>OCH<sub>2</sub>O, 15<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, September 4-6, **2012**.

8. **Adel Reisi-Vanani**, S. Hoseinpour, Ab initio studies on the reactivity and thermal decomposition of the  $\text{CF}_3\text{OCH}_2\text{O}$  radical, 15<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, Tehran, September 4-6, **2012**.
9. M. Hamadani, **A. Reisi-Vanani**, P. Razi, S. Hoseinifard, Study of photocatalytic behavior of photochemical doped  $\text{TiO}_2$  nanoparticles with In-V synthesized by sol-gel and hydrothermal methods, Nanomaterials: Applications and Properties, Sumy, Ukraine, September 17-22, **2012**.
10. **Adel Reisi-Vanani**, Masood Hamadani, Enhancement of the photocatalytic activity of doped and co-doped  $\text{TiO}_2$  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**.
11. Z. Tavangar, M. Hamadani, **A. Reisi-vanani**, Effect of calcination temperature on Preparation, Characterization and evaluation of photocatalytic activity of Sulfur doped  $\text{TiO}_2$  nanoparticles, 11<sup>th</sup> Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
12. M. Hamadani, **A. Reisi-vanani**, Synthesis, characterization and effect of calcinations temperature on phase transformation and photocatalytic activity of Cu,S-codoped  $\text{TiO}_2$  nanoparticles, 11<sup>th</sup> Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2010**.
13. **Adel Reisi-Vanani**, Masood Hamadani, Sol-gel preparation of Cu,S-codoped  $\text{TiO}_2$  nanoparticles and evaluation of phase transformation and photocatalytic activity, 13<sup>th</sup> Iranian Seminar of Physical Chemistry, Shiraz University, April **2010**.
14. **Adel Reisi-Vanani**, Masood Hamadani, Effect of calcination temperature on preparation, phase transformation and photocatalytic activity of S- $\text{TiO}_2$  nanoparticles, First Seminar of responsibility of basic science in Nanotechnology, Imam Hosein University, Tehran, December **2009**.
15. **Adel Reisi-Vanani**, Masood Hamadani, Preparation and characterization of Co- $\text{TiO}_2$  nanoparticles and optimize Co content to degradation of methyl orange under UV and Visible irradiation, First Seminar of responsibility of basic science in Nanotechnology, Imam Hosein University, Tehran, December **2009**.

16. **Adel Reisi-Vanani**, Masood Hamadanian, Preparation and characterization of pure TiO<sub>2</sub> nanoparticles, doping with Co, S and Fe-S and evaluation of photocatalytic activity to degradation of methyl orange and methylene blue under UV and Visible irradiation, 6<sup>th</sup> Student Seminar of Nanotechnology, Shahid Beheshti University of Medical Sciences, Tehran, December **2009**.
17. Masood Hamadanian, **Adel Reisi-Vanani**, Preparation and Characterization of Fe, S and Fe-S co-Doped TiO<sub>2</sub>, Nanoparticles and Evaluation of Photocatalytic Activity, 10<sup>th</sup> Netherlands Catalysis and Chemistry Conference, Leiden, Noordwijkerhout, March **2009**.