#### **Personal Data**

Name: Zahra Tavangar

Birth Date: March 22, 1972

Place of Birth: Zarin Shahr, Isfahan I.R. IRAN

**Nationality:** Iranian

Marital Status: Married

Children: One child

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I.R. IRAN. Tel.: +98-361-5912366 Fax: +98-361-5912397

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### **University Education**

2003-2009: Ph.D. Studies in Chemistry (computational chemistry)

Title: Molecular Dynamic Simulation of Fluid Flow Through Carbon Nanotube Junctions

Department of Chemistry, Faculty of Science, Isfahan University, Isfahan, I.R. IRAN

1994-1997: M.Sc. Studies in Chemistry (Physical Chemistry)

Title: Direct Determination of the Intermolecular Potential of Kr-N2, Xe-N2 and He-SF6 From The Extended

Principle of Corresponding States

Department of Chemistry, Faculty of Science, Bu-Ali Sina, Hamedan, I.R. IRAN

1990-1994: B.Sc. Studies in Chemistry (Pure Chemistry)

Department of Chemistry, Faculty of Science, University of Isfahan, Isfahan, I.R. IRAN

### Work Experience

2005-2008: General Chemistry and Physical Chemistry (courses and labs)

Payam-e-Noor University of Delijan, Delijan, I.R. IRAN

2009-2011: Physical Chemistry and Quantum Chemistry lecturer (courses and labs)

Kashan University, Kashan, I.R. IRAN

# **Teaching Experience**

#### Undergraduate Level

- 1- General Chemistry I & II and Its Laboratory
- 2- Physical Chemistry I & II and Its Laboratory
- 3- Computer in Chemistry

#### Postgraduate Level

1- Advanced Physical Chemistry



2- Quantum Chemistry I

### **Research Experience**

- 1- Computational Chemistry
- 2- Molecular Dynamic simulation
- 3- Intermolecular potensial
- 4- Transport property of Nano fluides

### **Publications:**

## A) Journal Papers

1- 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), 4296-4299.

2- H. Iloukhani, Z. Tavangar, E. K. Goharshadi,

"Direct determination of the intermolecular potential of Kr - N<sub>2</sub>, Xe - N<sub>2</sub> and He - SF<sub>6</sub> from the extended principle of corresponding states"

*Indian Journal of Chemistry A*, 40 (2001), 185-187.

3- H. Sabzyan, Z. Tavangar,

"Characterization of the flow of the CO/CO<sub>2</sub> gases through carbon nanotube junctions using molecular dynamic simulations"

Chemical Physics, 362 (2009), 120-129.

4- A. R. Ashrafi, M. Hamadanian, Z. Tavangar, H. Sabzyan,

"Symmetry of a capped nanotube"

Digest Journal of Nanomaterials and Biostructures, 4 (2009), 319-322.

### C) Conference Papers

1- 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.

2- 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.

3- 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.

4- H. Sabzyan, Z. Tavangar,

"MOLECULAR DYNAMIC SIMULATION OF THE FLOW OF THE CO/CO<sub>2</sub> GASES THROUGH CARBON NANOTUBE JUNCTION"

Proceeding of The Forth Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 12-15 July 2010.

5- H. Sabzyan, Z. Tavangar,

"A computational study of molecular transport through carbon nanotube"

Proceeding of The 13<sup>th</sup> Irainian Physical Chemistry Seminar, Shiraz, Iran, April 12-15, 2010.

6- - H. Sabzyan, Z. Tavangar,

"A computatuonal study of molecular transport through carbon nanotube"

Proceeding of The 14<sup>th</sup> Iranian Physical Chemistry Conference, University of Tehran, kish, 25-28 February 2011.

7- 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.

8- 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.