

Curriculum Vitae



Dr. Mohammad Chahkandi

Place and Date of Birth: Mashhad, Iran, 22 June, 1979.
Associate Prof. in Inorganic Chemistry
Dept. of Chemistry
Hakim Sabzevari University
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Academic and professional career:

- 2013 Ph.D.**, Inorganic Chemistry (Development and Suggestion of New Vanadium Bromoperoxidase Functional Models within Tripodal Amine Ligands: Theoretical Calculations Study with Prof. Dr. H. Eshtiagh-Hosseini and Prof. Dr. M. Hossein-Dokht), Ferdowsi University of Mashhad, Iran.
- 2010 Visiting Sabbatical of Ph.D. Program** with Prof. Dr. Winfried Plass, Friedrich Schiller University, Jena, Germany.
- 2006 M.Sc.**, Inorganic Chemistry (Synthesis of Sol-Gel-derived Hydroxyapatite and Evaluation of Effects of Various Sol-Gel Process on its Purity” with Prof. Dr. H. Eshtiagh-Hosseini and Prof. Dr. M. Hossein-Dokht), Ferdowsi University of Mashhad, Iran.
- 2003 B.Sc.** Applied Chemistry (Synthesis of Emulsion Poly (vinyl acetate)” with Prof. Dr. G. Zohuri), Ferdowsi University of Mashhad, Iran.

Professional Appointments:

- Assistant Professor, Hakim Sabzevari University, Iran, September 2013–November 2019.
- Associate Professor, Hakim Sabzevari University, Iran, November 2019–present.

Honors and Awards:

- Top researcher in Hakim Sabzevari University, Iran, 2019.
- Named in the World's Top 2% Scientists, 2020.

Main research interests:

- **Nanophotocatalyst**
 - Synthetization and fabrication of Hydroxyapatite bioceramic, Zeolites (natural and artificial), carbon-based compounds (GO, rGO, and g-C₃N₄), and Bi based perovskite in nano powders.
 - Compositd MOFs (UIO and ZIF) with CQdots for environmental applications
 - Electrochemistry deposition of the mentioned thin films for photocatalytic studies
 - Sustainable Environmental Chemistry:
Photocatalytic pollutants (drugs, dyes, phenols, antibiotic) degradation, Water splitting, H₂-generation, Advanced Oxidation Process (AOPs)
- **Quantum Theoretical Chemistry**
 - Molecular and electronic structural studies of new organic and coordination compounds
 - Spectroscopic and energetically considerations
 - Theoretical Crystal Engineering:
Binding energies of the involved non-covalent interactions
Total stabilization energies of pertinent crystalline network
Comparing the role of functionalized ligands in network stabilization
 - Kinetic and Transition states study of the chemical reactions (Haloperoxidases model vanadium complexes)

Publications:

- Author and co-author of more than 50 scientific ISI papers, 2 book chapters, and more than 30 international and national papers and abstracts.
- H-index: 16 (Google Scholar), i10-index: 20, Citation: 800 (Google Scholar).

List of Publication in Refereed Journals

1- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi “**Effects of Parameters of Sol-Gel Process on the Phase Evolution of Sol-Gel-derived Hydroxyapatite**”, *Materials Chemistry and Physics* 106 (2007) 310–316.

- 2- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi, A. Youssefi **“Preparation of anhydrous dicalcium phosphate, DCPA, through sol-gel process, identification and phase transformation evaluation”** *J. of Non – Crys. Sol.* 354 (2008) 3854–3857.
- 3- A.R. Salimi, M. Mirzaei, M. Chahkandi, A. Azadmehar, H. Eshtiagh-Hosseini, H. R. Khavasi, M. M. Amini. **“Experimental and theoretical studies of the triphenyltin(IV) chloride adduct of pyridine-2-ethanol”** *J. of Molecular Structure* 937 (2009) 44-49.
- 4- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi, A. Morsali **“A density functional theory investigation of the bromide oxidation mechanism by a vanadium bromoperoxidase model complex”** *Transition Met Chem.* 35 (2010) 939-947.
- 5- Mirzaei, M.; Eshtiagh-Hosseini, H.; Chahkandi, M.; Alfi, N.; Shokrollahi, A.; Shokrollahi N.; Janiak, A. **“Comprehensive Studies of Non-Covalent Interactions within Four New Cu(II) Supramolecules”** *CrystEngComm.* 14 (2012) 8468-8484.
- 6- Mirzaei, M.; Eshtiagh-Hosseini, H.; Mohammadi Abadeh, M.; Chahkandi, M.; Frontera A.; Hassanpoor, A. **“Influence of accompanying anions on supramolecular assembly and coordination geometry in Hg(II) complexes with 8-aminoquinoline: Experimental and theoretical studies”** *CrystEngComm.* 15 (2013) 1404-1413.
- 7- H. Eshtiagh-Hosseini, M. Chahkandi, M. Housain Dokht, M. Mirzaei **“Bromide Oxidation Mechanism by Vanadium Bromoperoxidase Functional Models with New Tripodal Amine Ligands: A Comprehensive Theoretical Calculations Study”** *Polyhedron.* 60 (2013) 93-101.
- 8- B. Chahkandi, S. F. Tayyari, M. Bakhshaei, M. Chahkandi **“Investigation of simple and water assisted tautomerism in a derivative of 1,3,4-oxadiazole: A DFT study”** *Journal of Molecular Graphics and Modelling* 44 (2013) 120–128.
- 9- B. Chahkandi, M. Mirzaei, M. Chahkandi, A. Shokrollahi, F. Zarghampour, M. Shamsipur **“Potentiometric and spectroscopic studies of three new mixed inorganic–organic hybrid materials based on Preyssler and Wells–Dawson heteropolyoxometalates containing proline, leucine, and asparagine”** *Journal of Iranian Chemical Society* 11 (2014) 187-198.
- 10- H. Eshtiagh-Hosseini, M. Mirzaei, M. Biabani, V. Lippolis, M. Chahkandi, and C. Bazzicalupi **“Insight into the connecting roles of interaction synthons and water clusters within different transition metal coordination compounds of pyridine-2,5-dicarboxylic acid: experimental and theoretical studies”** *CrystEngComm.* 15 (2013) 6752-6768.
- 11- B. Chahkandi, M. Chahkandi, B. Ashrafi **“Conformational Analysis of N- and C-Terminally Protected Tripeptide Model Glycyl-Isoleucine-Glycyl: An ab initio and DFT Study”** *Physical Chemistry Research.* 2 (2014) 68-75.
- 12- M. Chahkandi, **“Theoretical investigation of non-covalent interactions and spectroscopic properties of a new mixed-ligand Co(II) complex”** *Journal of Molecular Structure.* 1111 (2016) 193–200.

- 13- M. Chahkandi, "**⁵¹V NMR, ¹⁷O NMR, and UV–Vis computational studies of new VBPO functional models: Bromide oxidation reaction**" *Polyhedron* 109 (2016) 92–98.
- 14- M. Chahkandi, B. Madani Khoshbakht, M. Mirzaei, "**A theoretical study of intramolecular H–bonding and metal–ligand interactions in some complexes with bicyclic guanidine ligands**" *Computational and Theoretical Chemistry* 1095 (2016) 36–43.
- 15- M. Chahkandi, M. Mirzaei, "**Structural and particle size evolution of sol–gel-derived nanocrystalline hydroxyapatite**" *Journal of Iranian Chemical Society* 14 (2017) 567–575.
- 16- M. Chahkandi, H. A. Rahnamaye Aliabad, "**Evaluation of Non-covalent Binding Energies and Optoelectronic Properties of New CuBr₂(C₆H₇N)₂ Complex: DFT Approaches**" *Z. Anorg. Allg. Chem.* 643 (2017) 180–191.
- 17- U. Yunus, S. Ahmed, M. Chahkandi, M. H. Bhatti, M. Nawaz Tahir, "**Synthesis and theoretical studies of non–covalent interactions within a newly synthesized chiral 1,2,4-triazolo[3,4-b][1,3,4]thiadiazine**" *Journal of Molecular Structure* 1130 (2017) 688–698.
- 18- A. Amiri, M. Chahkandi, A. Targhoo, "**Synthesis of nano-hydroxyapatite sorbent for microextraction in packed syringe of phthalate esters in water samples**" *Analytica Chimica Acta*, 950 (2017) 64–70.
- 19- M. Chahkandi, M. H. Bhatti, U. Yunus, S. Shaheen, M. Nadeem, M. Nawaz Tahir, "**Synthesis and comprehensive structural studies of a novel amide based carboxylic acid derivative: Non–covalent interactions**" *Journal of Molecular Structure* 1133 (2017) 499–509.
- 20- H. A. Rahnamaye Aliabad, M. Chahkandi "**Comprehensive SPHYB and B3LYP-DFT Studies of Two Types of Ferrocene**" *Z. Anorg. Allg. Chem.* 643 (2017) 420–431.
- 21- M. Chahkandi, "**Mechanism of Congo red adsorption on new sol-gel-derived hydroxyapatite nano-particle**" *Materials Chemistry and Physics* 202 (2017) 340–351.
- 22- H. A. Rahnamaye Aliabad, M. Chahkandi "**Optoelectronic and structural studies of a Ni(II) complex including bicyclic guanidine ligands: DFT calculations**" *Computational and Theoretical Chemistry* 1122 (2017) 53–61.
- 23- M. Chahkandi, M. H. Bhatti, U. Yunus, N. Rehman, M. Nadeem, M. Nawaz Tahir, M. Zakria, "**Novel cocrystal of N-phthaloyl-L-alanine with 2,2'-bipyridyl: Synthesis, computational and free radical scavenging activity studies**" *Journal of Molecular Structure* 1152 (2018) 1–10.
- 24- Z. Rahmati, M. Mirzaei, M. Chahkandi, J. T. Mague, "**Accurate DFT studies on crystalline network formation of a new Co(II) complex bearing 8-aminoquinoline**" *Inorg. Chim. Acta.* 473 (2018) 152-159.

25- M. Chahkandi, H. A. Rahnamaye Aliabad, **"Role of hydrogen bonding in establishment of a crystalline network of Cu (II) complex with hydrazon-derived ligand: optoelectronic studies"** *Chemical Papers* 72 (2018) 1287-97.

26- M. Chahkandi, A. Amiri, S.R. Saadatdar Arami, **"Extraction and preconcentration of organophosphorus pesticides from water samples and fruit juices utilizing hydroxyapatite/Fe₃O₄ nanocomposite"** *Microchemical Journal* 144 (2019) 261-269.

27- H. A. Rahnamaye Aliabad, M. Chahkandi, **"Theoretical study of crystalline network and optoelectronic properties of erlotinib hydrochloride molecule: non-covalent interactions consideration"** *Chemical Papers* 73 (2019) 737-46.

28- M. Chahkandi, S.R. Saadatdar Arami, M. Mirzaei, B. Mahdavi, S.M. Hosseini Tabar, **"A new effective nano-adsorbent and antibacterial material of hydroxyapatite"** *Journal of Iranian Chemical Society* 16 (2019) 695-705. DOI: <https://doi.org/10.1007/s13738-018-1546-1>.

29- M. Chahkandi, M. H. Bhatti, U. Yunus, M. Nadeem, N. Rehman, M. Nawaz Tahir **"Crystalline network study of new N-phthaloyl-b-Alanine with benzimidazole, cocrystal: Computational consideration & free radical scavenging activity"** *Journal of Molecular Structure* 1191 (2019) 225–236.

30- M. Chahkandi, B. Chahkandi **"A New Mixture of Nano-structure of Potassium-incorporated Hydroxyapatite/ β -tricalcium Phosphate/calcium Pyrophosphate"** *Inorg. Chem. Res.* 2(1) (2019) 6-15.

31- M. Chahkandi, H. A. Rahnamaye Aliabad **"Crystalline network form of Gefitinib molecule stabilized by non-covalent interactions: DFT–D calculations"** *Chemical physics* 525 (2019). DOI: <https://doi.org/10.1016/j.chemphys.2019.110418>.

32- M. Chahkandi, M. Zargazi, **"Novel method of Square Wave Voltammetry for deposition of Bi₂S₃ thin film: Photocatalytic reduction of hexavalent Cr in single and binary mixtures"** *Journal of Hazardous Materials* 380 (2019) DOI: doi.org/10.1016/j.jhazmat.2019.120879.

33- B. Maleki, M. Chahkandi, R. Tayebee, S. Kahrobaei, S. Hemmati **"Synthesis and Characterization of Nanocrystalline hydroxyapatite and its Catalytic Behavior towards Synthesis of 3,4-Disubstituted Isoxazole-5(4H)-ones in Water"** *Applied Organometallic Chemistry* 33 (10) (2019). DOI: <https://doi.org/10.1002/aoc.5118>.

34- M. Chahkandi, A. Amiri, **"Hydroxyapatite/Fe₃O₄ nanocomposite as efficient sorbent for the extraction of phthalate esters from water samples"** *Inorg. Chem. Res.* 2(1) (2019) 50-64.

35- M. Chahkandi, M. Zargazi, **"New water based EPD thin BiVO₄ film: Effective photocatalytic degradation of Amoxicillin antibiotic"** *Journal of Hazardous Materials* 389 (2019) 121850, DOI: [10.1016/j.jhazmat.2019.121850](https://doi.org/10.1016/j.jhazmat.2019.121850).

- 36- HA Rahnamaye Aliabad, M Chahkandi, "Investigation of Non-Covalent Interactions and Optical Properties in a Manganese (II) Complex with Pyridine-N-oxide-2-carboxylic Acid" *Nashrieh Shimi va Mohandesi Shimi Iran* 40 (2) (2021) 195-207.
- 37- S. N. Vakili, M. Rezayi, M. Chahkandi, Z. Meshkat, M. Fani, A. Moattari "A novel electrochemical DNA biosensor based on hydroxyapatite nanoparticles to detect BK polyomavirus in the urine samples of transplant patients" *IEEE Sensors Journal* (2020) DOI: 10.1109/JSEN.2020.2982948.
- 38- F. Narenji-Sani, R. Tayebee, M. Chahkandi "New Task-Specific and Reusable ZIF-like Grafted H6P2W18O62 Catalyst for the Effective Esterification of Free Fatty Acids" *ACS Omega* 5 (2020) 9999–10010.
- 39- B. Chahkandi, M. Chahkandi "A reconnaissance DFT study of the full conformational analysis of N-formyl-L-serine-L-alanine-NH₂ dipeptide" *Journal of Molecular Modeling* 26(151) (2020), DOI: 10.1007/s00894-020-04382-9.
40. S. Sheikh, M. A. Nasser, M. Chahkandi, A. Allahresani, O. Reiser "Functionalized magnetic PAMAM dendrimer as an efficient nanocatalyst for a new synthetic strategy of xanthene pigments" *Journal of Hazardous Materials* (2020) 122985, DOI: 10.1016/j.jhazmat.2020.122985.
41. M. Chahkandi, A. Keivanloo Shahrestanaki, M. Mirzaei, M. N. Tahir, J. T. Mague "Crystal and molecular structure of [Ni(2-H₂NC(=O)C₅H₄N)₂(H₂O)₂][Ni(2,6-(O₂C)₂C₅H₃N)₂].4.67H₂O; DFT studies on hydrogen bonding energies in the crystal" *Acta Crystallographica Section B* (2020) B76, 591–603, DOI: 10.1107/S2052520620006472.
42. R. Tayebee, E. Esmaili, B. Maleki, A. Khoshniat, M. Chahkandi, N. Mollania "Photodegradation of methylene blue and some emerging pharmaceutical micropollutants with an aqueous suspension of WZnO-NH₂@H3PW12O₄₀ nanocomposite" *Journal of Molecular Liquids* (2020) 10.1016/j.molliq.2020.113928.
43. M. Chahkandi, M. Zargazi, "Water EPD based of 2D-Bi₂WO₆ ultrathin film on innovative designed substrates: Efficient photocatalytic degradation of binary antibiotics" *Journal of Molecular Liquids* 335 (2021) 116153, DOI: 10.1016/j.molliq.2021.116153.
44. K. Salimiyan Rizi, Z. Meshkat, M. Chahkandi, M. Gholami, M. Sankian, K. Ghazvini, H. Farsiani, E. Aryan, and M. Rezayi, "A PCR-Free Genome Detection of Mycobacterium Tuberculosis Complex in Clinical Samples using MWCNT/PPy/KHApNps Modified Electrochemical Nano-Biosensor" *Journal of The Electrochemical Society* 168 (2021) 077501. DOI: 10.1149/1945-7111/ac0b29.
45. M. Chahkandi, M. Zargazi, A. Ahmadi, E. Koushki, A. Ghasedi, "In-Situ synthesis of holey g-C₃N₄ nanosheets decorated by Hydroxyapatite nanospheres as efficient visible light photocatalyst" *RSC Advances* 11 (2021) 31174-31188. DOI: 10.1039/d1ra05259d.

46. M. Chahkandi, M. Zargazi, A. Hajizadeh, R. Tayebee, **“In-situ incorporation of Bi₂O₃ nanorods and Ag metal plasmonic surface into crystalline HAp nanosheets: Efficient visible light degradation of phenol”** *J. Alloys and Comps.* 902 (2022) 163737. DOI: 10.1016/j.jallcom.2022.163737.

47. S. Sheikh, M. A. Nasser, M. Chahkandi, O. Reiser, A. Allahresani, **“Dendritic structured palladium complexes: magnetically retrievable, highly efficient heterogeneous nanocatalyst for Suzuki and Heck cross-coupling reactions”** *RSC Advances* 12 (2022) 8833-8840. DOI: 10.1039/d2ra00487a.

48. M. Zargazi, M. Chahkandi, M. Baghayeri, **“New highly efficient 2D/1D HAp/g-C₃N₄ photocatalyst thin film insight into crystal orientation and C-vacancy effects”** *Chemosphere*, 303(2) (2022) 135079. DOI: 10.1016/j.chemosphere.2022.135079.

BOOK CHAPTERS:

1- M. Chahkandi, M. Zargazi, **“Nanomaterials for the photoremediation of pollutants”** in the book edition **“Water Pollution and Remediation: Photocatalysis”** by Springer, Inamuddin, M.I. Ahamed, E. Lichtfouse, (2021).

2- M. Zargazi, M. Chahkandi, **“Bismuth-based compounds as visible light photocatalyst for remediation and water splitting”** in the book edition **“Water Pollution and Remediation: Photocatalysis”** by Springer, Inamuddin, M.I. Ahamed, E. Lichtfouse, (2021).

Publication in conference proceedings

1- S. Amiri, M. Chahkandi, M. Zargazi, **“Efficient thin film photocatalyst of UiO-66/Ag₂O heterojunction within Cr(VI) reduction reaction”** in proceeding of the 21st ICS International Chemistry Conference, Azarbaijan Shahid Madani University, Tabriz, Iran, 2022.

2- V. Sokhanvaran, F. Azimi, B. Maleki, M. Chahkandi, **“Theoretical Investigation of 2,3,4,6,7,8,9,10 Octahydropyrimido[1,2-*a*]azepinium Halids”** in proceeding of the 27th Iranian Conference on Organic Chemistry, Urmia University, Iran, 2019.

3- V. Sokhanvaran, F. Azimi, B. Maleki, M. Chahkandi, **“DFT Study of Bis-2,3,4,6,7,8,9,10-Octahydropyrimido[1,2-*a*]azepiniummethyl Disulfate [DBU]₂[EDS]”** in proceeding of the 27th Iranian Conference on Organic Chemistry, Urmia University, Iran, 2019.

4- M. Chahkandi, **“Effective nano-catalysts for polluters and pesticides photo-remediation”** in proceeding of the 6th Iranian National Zeolite Conference, Quchan University of Technology Quchan, Iran, 2019. (As Keynote Speaker).

5- M. Chahkandi, M. Zargazi, A. Ahmadi, **“Enhanced photocatalytic performance over new nano structure of HAp/g-C₃N₄: Methylene Blue photodegradation study”** in

proceeding of the 20th Inorganic Chemistry Conference of Iran, University of Sistan and Baluchestan, Zahedan, Iran, 2019.

6- M. Chahkandi, M. Zargazi, A. Ahmadi, **“Novel *p-n* heterojunction of Ag/HAp/g-C₃N₄ photocatalyst: study the efficient photocatalytic performance for phenol degradation”** in proceeding of the 20th Inorganic Chemistry Conference of Iran, University of Sistan and Baluchestan, Zahedan, Iran, 2019.

7- M. Chahkandi, R. Tayebee, M. R. Meisami, **“The electronic and molecular structures of some new Cu(II) complexes with tripodal amine ligands: DFT studies”** in proceeding of the 20th Inorganic Chemistry Conference of Iran, University of Sistan and Baluchestan, Zahedan, Iran, 2019.

8- M. A. Nasser, S. Sheikh, A. Allahresani, M. Chahkandi, **“Synthesis Co-Complex Supported in Surface γ -Fe₂O₃ and Application in Suzuki–Miyaura Cross Coupling Reaction”** in proceeding of the 7th International Congress on Nanoscience and Nanotechnology (ICNN 2018), Tehran, Iran, 2018.

9- M. A. Nasser, S. Sheikh, A. Allahresani, M. Chahkandi, **“Cobalt Complex Supported Magnetic Nanoparticles: As a New Catalyst for C–C Bond Formation via Suzuki-Miyaura Cross-Coupling Reaction”** in proceeding of the 7th International Congress on Nanoscience and Nanotechnology (ICNN 2018), Tehran, Iran, 2018.

10- A. Hajizadeh, M. Chahkandi, **“New efficient visible light photocatalyst for degradation of phenol: Nano-particle of HAP/Bi₂O₃-Ag composite”** in proceeding of the 20th Iranian Chemistry Congress, Mashhad, Iran, 2018.

11- M. Chahkandi, **“New nano-structure of potassium-substituted hydroxyapatite/ β -TCP/PPP mixture”** in proceeding of the 6th Biennial International Conference on Ultrafine Grained and Nanostructured Materials (UFGNSM2017), Kish Island, Iran, 2017.

12- M. Chahkandi, M. Ebrahimi, **“A newly synthesized proton transfer ligand with 2, 6-pyridine dicarboxylic acid and pyridine-3-carboxamide: Characterization and DFT study”** in proceeding of the 19th Inorganic Chemistry Conference of Iran, Chemistry and Chemical Engineering Centre of Iran, Tehran, Iran, 2017.

13- M. Chahkandi, M. Ebrahimi, **“Synthesis and characterization of a new Cu(II) proton transfer complex with 2,6-pyridine dicarboxylic acid and 3-(aminocarbonyl)pyridine”** in proceeding of the 19th Inorganic Chemistry Conference of Iran, Chemistry and Chemical Engineering Centre of Iran, Tehran, Iran, 2017.

14- M. Chahkandi, S.R. Saadatdar Arami, **“New sol-gel-derived Na-substituted hydroxyapatites nanoparticles”** in proceeding of the 18th Inorganic Chemistry Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, 2017.

15- M. Chahkandi, S.R. Saadatdar Arami, **“Na-doped hydroxyapatite as efficient adsorbent for removal of Congo red dye from aqueous solution”** in proceeding of the 18th

Inorganic Chemistry Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, **2017**.

16- M. Chahkandi, F. Mohammadi Zonoz, B. Madani Khoshbakht, **“Investigation of Hydrogen bond within some Fe and Ni complexes: A DFT study”** in proceeding of the 17th Inorganic Chemistry Conference of Iran, Shahid Madani University, Tabriz, Iran, **2015**.

17- M. Chahkandi, F. Mohammadi Zonoz, B. Madani Khoshbakht, **“Study of Hydrogen bond in some Fe and Ni complexes with NMR and NBO calculations”** in proceeding of the 17th Inorganic Chemistry Conference of Iran, Shahid Madani University, Tabriz, Iran, **2015**.

18- M. Chahkandi, F. Mohammadi Zonoz, Z. Akbari Ghane, M. Akbari, **“The vibrational and UV-Vis spectroscopic and NBO studies of four new Cu(II) complexes with dicarboxylic ligands: A DFT study”** in proceeding of the 16th Inorganic Chemistry Conference of Iran, Bu-Ali Sina University, Hamedan, Iran, **2014**.

19- M. Chahkandi, F. Mohammadi Zonoz, Z. Akbari Ghane, M. Akbari, **“⁶³Cu NMR computational study of some new Cu complexes containing dicarboxylic ligands”** in proceeding of the 16th Inorganic Chemistry Conference of Iran, Bu-Ali Sina University, Hamedan, Iran, **2014**.

20- M. Chahkandi, F. Mohammadi Zonoz, Z. Akbari Ghane, M. Akbari, **“Structural and electronic properties of three new Cu(II) complexes with carboxylic ligands: A DFT study”** in proceeding of the 3rd National Conference on New Technologies in Chemistry and Chemical Engineering, Ghoochan Branch, Islamic Azad University, Iran, **2014**.

21- M. Chahkandi, **“Particle size evaluation of Sol-Gel-derived nano-crystalline hydroxyapatite powders by XRD and TEM methods”** in proceeding of the 15th Inorganic Chemistry Conference of Iran, Hakim Sabzevari University, Sabzevar, Iran, **2013** (lecture).

22- M. Chahkandi, **“⁵¹V-NMR and UV-Vis Computational Studies of VBPO Functional Models: Bromide Oxidation Reaction”** in proceeding of the 15th Inorganic Chemistry Conference of Iran, Hakim Sabzevari University, Sabzevar, Iran, **2013**.

23- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi, A. Morsali. **“Reactivity and mechanism of bromide oxidation by vanadium bromoperoxidase functional model complexes: A DFT study”** in proceeding of the 12th Inorganic Chemistry Conference of Iran, Rasht, **2010** (lecture).

24- B. Chahkandi, M. Chahkandi **“Amount evaluation of the adsorption of BSA protein onto the particles of Sol-Gel-derived Hydroxyapatite”**, in proceeding of the 6th National Biotechnology Congress of Iran, Tehran, Iran, **2009** (lecture).

25- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi, A. Morsali **“DFT investigation of bromide oxidation mechanism by [V(⁵⁺)O(O₂)H₂O]₂. Determination of reactive, transition state and product compounds”** in proceeding of the 11th Inorganic Chemistry Conference of Iran, Isfahan, **2009**.

26- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi **“Synthesis, Characterization and Phase purity evaluation of Hydroxyapatite powders by various Sol – Gel methods”**, in proceeding of the 9 th Iranian Inorganic Chemistry Conference, Semnan, Iran, **2007**.

27- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi **“Synthesis, Characterization and Phase Conversion evaluation of Anhydrous Dicalcium Phosphate (Monetite) by Sol – Gel method”**, in proceeding of the 9 th Iranian Inorganic Chemistry Congress, Semnan, Iran, **2007** (lecture).

28- H. Eshtiagh Hosseini, M. Housain Dokht, M. Chahkandi, M. Darrodi **“Evaluation of particle size of Sol-Gel-derived nanocrystalline Hydroxyapatite by Scherrer equation and Williamson-Hall curves”**, in proceeding of the 1th Nanotechnology Conference of Shiraz, Iran, **2007** (lecture).

29- H. Eshtiagh Hosseini, M. Housain Dokht, M. Darrodi, M. Chahkandi **“Synthesis and Characterization of nanocrystalline Hydroxyapatite powder and thin film by Sol-Gel method “**, in proceeding of the 1th Nanotechnology Conference of Shiraz, Iran, **2007**.

30- H. Eshtiagh Hosseini, M. Housain Dokht, A. Yousefi, M. Chahkandi, M. Darrodi **“Synthesis of high purity nano Hydroxyapatite powders by Sol-Gel method”**, in proceeding of the 4th Iranian Chemistry Conference Payame Noor University, Tabriz, Iran, **2006**.

31- B. Chahkandi, M. Monajemi, M. Chahkandi, A. Amiri, S. Ketabi. **“Abinitio and DFT Study of the Effect of the Dielectric Constant of Solvent on Hydrogen Bonding in Different Configurations of Adenine-Thymine Base Pairs with PCM: Comparison and Analysis with Gas phase”**, in proceeding of the 11th International Chemistry Congress of Asia, Seoul University, Korea, **2005**.