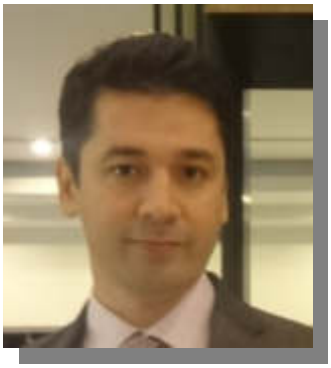
Curriculum Vitae



Dr. Mohammad Chahkandi

Place and Date of Birth: Mashhad, Iran, 22 June, 1979.
Associate Prof. in Inorganic Chemistry
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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-C_3N_4), and Bi based perovskite in nano powders.
  - Composited 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, H_2-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: 820 (Google Scholar).

List of Publication in Refereed Journals

1- H. Eshtiagh Hossseini, 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 Hossseini, 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. Azadmeher, 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 Hossseini, 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 aspargine"** *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, **"^{51}V NMR, ^{17}O 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-b-alanine with 2,2ebipyridyl: 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 Bi_2S_3 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/Fe_3O_4 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.

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. Nasseri, 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 $[Ni(2\text{-}H_2NC(=O)C_5H_4N)_2(H_2O)_2][Ni(2,6\text{-}(O_2C)_2C_5H_3N)_2]\cdot 4.67H_2O$; 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. Esmaeili, 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–C_3N_4 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. Nasseri, 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.

49. D. Khademi, M. Zargazi, M. Chahkandi, M. Baghayeri, "**A novel γ–BMO@BMWO Z–Scheme heterojunction for promotion photocatalytic performance: nanofibers thin film by Co–axial–electrospun"** *Environmental Research*, 219 (2023) 115154. DOI: 10.1016/j.envres.2022.115154

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/Ag_2O 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*]azepiniumethyl 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-C_3N_4: 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-C_3N_4 photocatalyst: study the efficient photocatalystic 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. Nasseri, 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. Nasseri, 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/CPP 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 dicarboxilic 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 Engeeniering, 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 Hossseini, 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 Hossseini, M. Housain Dokht, M. Chahkandi, A. Morsali **"DFT investigation of bromide oxidation mechanism by [V($^{5+}$)O(O2)Hheida]. Determination of reactive, transition state and product compounds"** in proceeding of the 11th Inorganic Chemistry Conference of Iran, Isfahan, **2009**.

26- H. Eshtiagh Hossseini, 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 Hossseini, 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 Hossseini, 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 Hossseini, 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 Hossseini, 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**.