

PERSONAL INFORMATION



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POSITION

Associate Professor of Physical Chemistry (Molecular Modeling and Simulations)-Materials Science and Nanotechnology Department, Faculty of Postgraduate Studies for Advanced Sciences (PSAS), Beni-Suef University, Beni-Suef, Egypt.

EDUCATION

- [01/2013-05/2014] Post-Doctor Fellow, Chemistry Dept., University of Aveiro, Portugal.
- [03/2010-12/2012] Post-Doctor Fellow, Chemical Engineering Dept., NTUST, Taiwan.
- [01.2010] Ph.D. Physical Chemistry, National Taiwan University of Science and Technology (NTUST), Taiwan.
- [01.2005] M.Sc. Analytical Chemistry, Cairo University, Egypt.
- [06.1999] B.Sc. Chemistry, Cairo University, Beni-Suef, Egypt.

Honours and awards

1. Prof. Y. P. Shih Paper Award, Taiwan Institute of Chemical Engineers, Taiwan, 2017.
2. Misr el Kheir Foundation, Scientific Publications Award, Egypt, 2010

Teaching

Faculty of Postgraduate Studies for Advanced Sciences:

1. NT605 Modelling & Simulation
2. NT510 Nanomaterials for Catalysis
3. NT604 Instrumental Analysis
4. NT512 Applied Physical Chemistry

Faculty of Navigation Sciences and Space Technology

5. SNS 307, Thermodynamics

Faculty of Earth Science

6. Thermodynamics

WORK EXPERIENCE

- [06/2017- 09/2022] Lecturer, Materials Science and Nanotechnology Dept., Faculty of Postgraduates for Advanced Sciences (PSAS), Beni-Suef University.
- [06/2017- till now] Lecturer, Materials Science and Nanotechnology Dept., Faculty of Postgraduates for Advanced Sciences (PSAS), Beni-Suef University.
- [2002-2017] Occupational Safety & Health, Directorate of Manpower and Immigration, Beni-Suef.
- [08/2005-08/2007] Director of Planning & Evaluation, Arabian Fire Safety Academy, Kingdom of Saudi Arabia.

PUBLICATIONS (98)

1. HA Younes, **Mohamed Taha**, R Khaled, HM Mahmoud, RM Abdelhameed. Perovskite/Metal-Organic Framework photocatalyst: A novel nominee for eco-friendly uptake of pharmaceuticals from wastewater, *Journal of Alloys and Compounds*, **2023**, 930, 167322
2. **Mohamed Taha**, RA Abdelhay, MH Khedr. Vacancy defects transform zinc tellurite glass from insulator to semiconductor: A first-principles prediction, *Optik*, **2022**, 271, 170125
3. EK Mahmoud, AA Farghali, SI El-dek, **Mohamed Taha**. Structural stabilities, mechanical and thermodynamic properties of chalcogenide perovskite AB_3 (A= Li, Na, K, Rb, Cs; B= Si, Ge, Sn) from first-principles study, *European Physical Journal Plus*, **2022**, 137(9), 1006.
4. HH AbdElAziz, **Mohamed Taha**, WMA El Rouby, MH Khedr, L Saad. Evaluating the performance of $Cs_2PtI_6-xBr_x$ for photovoltaic and photocatalytic applications using first-principles study and SCAPS-1D simulation, *Heliyon*, **2022**, 8(10), e10808
5. H Samir, **Mohamed Taha**, SI El-Dek, AH Zaki. Electronic Structures and Electrical Properties of Cr^{2+} -, Cu^{2+} -, Ni^{2+} -, and Zn^{2+} -Doped Sodium Titanate Nanotubes, *ACS Omega*, **2022**, 7(31), pp. 27587–27601
6. SA Mahmoud, **Mohamed Taha**, ESH Khaled, WH Hassan, FI Abo El-Ela, AA Abdel-Khalek, RA Mohamed. Experimental and Molecular Modeling Studies on the Complexation of Chromium (III) with the Angiotensin-Converting Enzyme Inhibitor Captopril, *ACS Omega*, **2022**, , 7, 18, 15909–15918
7. HE Emam, M El-Shahat, **Mohamed Taha**, RM Abdelhameed. Microwave assisted post-synthetic modification of IRMOF-3 and MIL-68-NH₂ onto cotton for Fuel purification with computational explanation, *Surfaces and Interfaces*, **2022**, 30, 101940
8. HA Mohamedien, SM Kamal, AG El-Deen, **Mohamed Taha**, MM El-Deeb. Electrochemical and computational estimations of cephalosporin drugs as eco-friendly and efficient corrosion inhibitors for aluminum in alkaline solution, *Scientific Reports*, **2022**, 12(1), 13333
9. W Kamal, R Mahmoud, AE Allah, A Abdelwahab, **Mohamed Taha**, AA Farghali. Insights into synergistic utilization of residual of ternary layered double hydroxide after oxytetracycline as a potential catalyst for methanol electrooxidation, *Chemical Engineering Research and Design*, **2022**, 188, pp. 249–264

10. HA Mohamedien, SM Kamal, **Mohamed Taha**, MM EL-Deeb, AG El-Deen. Experimental and computational evaluations of cefotaxime sodium drug as an efficient and green corrosion inhibitor for aluminum in NaOH solution, *Materials Chemistry and Physics* **2022**, 290, 126546
11. Esraa A. Mansour, **Mohamed Taha**, R. K. Mahmoud, N. Shehata, R. M. Abdelhameed. Remarkable adsorption of oxygenated compounds from liquid fuel using copper-based framework incorporated onto kaolin: Experimental and theoretical studies, *Applied Clay Science*, **2022**, 216, 106371
12. Heba A.Younes, **Mohamed Taha**, R. Mahmoud, H. M. Mahmoud, R. M .Abdelhameed. High adsorption of sodium diclofenac on post-synthetic modified zirconium-based metal-organic frameworks: Experimental and theoretical studies, *Journal of Colloid and Interface Science*, **2022**, 607, 334-346.
13. R. M. Abdelhameed, **Mohamed Taha**, Hassan Abdel-Gawad, Hossam E. Emam. Purification of soybean oil from diazinon insecticide by iron-based metal organic framework: Effect of geometrical shape and simulation study, *Journal of Molecular Structure*, **2022**, 1250, 131914.
14. SA Mahmoud, **Mohamed Taha**, ESH Khaled, AA Abdel-khalek, RA Mohamed. Kinetics and mechanism of the oxidation of chromium (III) complex involving the antifibrinolytic drug Tranexamic acid by periodate, *Egyptian Journal of Chemistry*, **2022**,
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15. R. K. Mahmoud, **Mohamed Taha**, Amal Zaher, Rafat M. Amin. Understanding the physicochemical properties of Zn–Fe LDH nanostructure as sorbent material for removing of anionic and cationic dyes mixture, *Scientific Reports*, **2021**, 11, 21365.
16. S.A. Mahmoud, **Mohamed Taha**,* R.A. Mohamed, E.S.H. Khaled, A. Abdel-Abdel-khalek,* Complexation of chromium (III) with the antifibrinolytic drug tranexamic acid: Formation, kinetics, and molecular modeling studies, *Journal of Molecular Liquids*, **2021**, 329, 115513.
17. **Mohamed Taha**,* H. R. AbdEl-Mageed, M. J. Lee, DFT Study of cyclic glycine-alanine dipeptide binding to gold nanoclusters, *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107823.
18. N. Saikia, **Mohamed Taha**, R. Pandey, Molecular Insights on the Dynamic Stability of Peptide Nucleic Acid Functionalized Carbon and Boron Nitride Nanotubes, *Physical Chemistry Chemical Physics*, **2021**, 23, 219-228.
19. R. M. Abdelhameed,* **Mohamed Taha**,* H. Abdel-Gawad, B. Hegazi, Amino-functionalized Al-MIL-53 for dimethoate pesticide removal from wastewater and their intermolecular interactions, *Journal of Molecular Liquids*, **2021**, 327, 114852.
20. R. Saleh, A. H.Zaki, F. I. AboEl-Ela, A. A. Farghali, Mohamed Taha, R. Mahmoud, Consecutive removal of heavy metals and dyes by a fascinating method using titanate nanotubes, *Journal of Environmental Chemical Engineering*, **2021**, 9, 104726.
21. A Zaher, **Mohamed Taha**,* R.K. Mahmoud,* Possible adsorption mechanisms of the removal of tetracycline from water by La-doped Zn-Fe-layered double hydroxide, *Journal of Molecular Liquids*, **2021**, 322, 114546.
22. H.H. Kora, Mohamed Taha,* A Abdelwahab, A.A. Farghali, S. I. El-Dek*, Effect of pressure on the geometric, electronic structure, elastic, and optical properties of the normal spinel MgFe₂O₄: a first-

- principles study, *Materials Research Express*, **2020**, 7, 106101
23. H.H. Kora, **Mohamed Taha**,* A.A. Farghali, S.I. EL-Dek,* First-Principles Study of the Geometric and Electronic Structures and Optical Properties of Vacancy Magnesium Ferrite, *Metallurgical and Materials Transactions A* **2020**, 51, 5432–5443.
 24. A.H. Tiwikrama, **Mohamed Taha**, M.J. Lee, Experimental and computational studies on the solubility of carbon dioxide in protic ammonium-based ionic liquids, *Journal of the Taiwan Institute of Chemical Engineers*, **2020**, 112, 152-161.
 25. M. K. Abdel-Sattar and **Mohamed Taha**,* Electronic structures and optoelectronic properties of ATiOPO₄ (A = H, Li, Na, K, Rb, Cs, Fr, NH₄, Ag) compounds and their applications in water splitting, CO₂ reduction, and photo-degradation, *Materials Research Express* **2020**, 7, 045901.
 26. A. Zaher, **Mohamed Taha**,* A.A. Farghali, R.K. Mahmoud,* Zn/Fe LDH as a clay-like adsorbent for the removal of oxytetracycline from water: combining experimental results and molecular simulations to understand the removal mechanism, *Environmental Science and Pollution Research* **2020**, 27, 12256–12269.
 27. **Mohamed Taha*** and M.-J. Lee, Influence of the alanine side-chain methyl group on the peptide-gold nanoparticles interactions, *Journal of Molecular Liquids* **2020**, 302, 112528.
 28. G.Y. Abo El-Reesh, A.A. Farghali, **Mohamed Taha**, R.K. Mahmoud,* Novel synthesis of Ni/Fe layered double hydroxides using urea and glycerol and their enhanced adsorption behavior for Cr(VI) removal, *Scientific Reports* **2020**, 10, 587.
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 33. R.M. Amin,* **Mohamed Taha**, S.A. Abdel Moaty, F.I. Abo El-Ela, H.F. Nassar, Y. GadelHak, R.K. Mahmoud. Gamma radiation as a green method to enhance the dielectric behaviour, magnetization, antibacterial activity and dye removal capacity of Co–Fe LDH nanosheets, *RSC Advances* **2019**, 9, 32544–32561.
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35. **Mohamed Taha*** and H.F. Nassar, Molecular design of mass-separating agents for separation of cyclic ethers and acetonitrile from water, *Journal of Molecular Liquids* **2019**, 281, 324-331.
36. **Mohamed Taha*** and M.-J. Lee, Does the peptide backbone unit interact with gold nanoclusters? Insights from computational modelling, *Journal of Biomolecular Structure and Dynamics* **2019**, 37, 4258–4266.
37. I. Ling, **Mohamed Taha**, N.A. Al-Sharji, O.K. Abou-Zied,* Selective binding of pyrene in subdomain IB of human serum albumin: Combining energy transfer spectroscopy and molecular modelling to understand protein binding flexibility, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2018**, 194, 36–44.
38. R.M. Abdelhameed, H. Abdel-Gawad, **Mohamed Taha,*** B Hegazi, Separation of bioactive chamazulene from chamomile extract using metal-organic framework, *Journal of Pharmaceutical and Biomedical Analysis* **2017**, 146, 126–134.
39. A. Rani, **Mohamed Taha**, P. Venkatesu,* M.-J. Lee, Coherent Experimental and Simulation Approach to Explore the Underlying Mechanism of Denaturation of Stem Bromelain in Osmolytes, *Journal of Physical Chemistry B* **2017**, 121, 6456–6470.
40. **Mohamed Taha**, M.V. Quental, F.A. Silva, E.V. Capela, M.G. Freire, S.P.M. Ventura, J.A.P. Coutinho,* Good's Buffer Ionic Liquids as Relevant Phase-Forming Components of Self-Buffered Aqueous Biphasic Systems, *Journal of Chemical Technology and Biotechnology*. **2017**, 92, 2287–2299.
41. B.S. Gupta, **Mohamed Taha**, M.-J. Lee,* A green process for recovery of 1-propanol/2-propanol from their aqueous solutions: Experimental and MD simulation studies, *Journal of Chemical Thermodynamics* **2017**, 105, 76-85.
42. S. Altway, **Mohamed Taha**, M.-J. Lee,* Phase Separation of Alcohol (1-Propanol, 2-Propanol, or tert-Butanol) from Its Aqueous Solution in the Presence of Biological Buffer MOPS, *J. Chem. Eng. Data* **2017**, 62, 2509–2515.
43. B.S. Gupta, M.Y. Fang, **Mohamed Taha**, M.-J. Lee,* Separation of 1,3-Dioxolane, 1,4-Dioxane, Acetonitrile and tert-Butanol from Their Aqueous Solutions by Using Good's Buffer HEPES-Na as an Auxiliary Agent, *Journal of the Taiwan Institute of Chemical Engineers* **2016**, 66, 43-53.
44. **Mohamed Taha**, J.A.P. Coutinho,* Organic-Phase Biological Buffers for Biochemical and Biological Research in Organic Media, *Journal of Molecular Liquids* **2016**, 221, 197–205.
45. **Mohamed Taha,*** Designing New Mass-Separating Agents Based on Piperazine-Containing Good's Buffers for Separation of Propanols and Water Azeotropic Mixtures using COSMO-RS Method, *Fluid Phase Equilibria* **2016**, 425, 40-46.
46. D. Hartanto, B.S. Gupta, **Mohamed Taha**, M.-J. Lee,* Isobaric Vapor-Liquid Equilibrium of tert-Butanol + Water System with Biological Buffer TRIS at 101.3. *Journal of Chemical Thermodynamics* **2016**, 98, 159-164.
47. B.S. Gupta, **Mohamed Taha**, M.-J. Lee,* Extraction of Active Enzyme by Self-Buffering Ionic Liquids: A Green Medium for Enzymatic Research, *RSC Advances* **2016**, 6, 18567-18576.
48. I. Khan, **Mohamed Taha**, S.P. Pinho, J.A.P. Coutinho,* Interactions of pyridinium, pyrrolidinium

- or piperidinium based ionic liquids with water: Measurements and COSMO-RS modelling, *Fluid Phase Equilibria* **2016**, 414, 93–100.
49. **Mohamed Taha**, I. Khan, J.A.P. Coutinho,* Complexation and Molecular Modeling Studies of Europium(III)-Gallic Acid-Amino Acid Complexes, *Journal of Inorganic Biochemistry* **2016**, 157, 25–33.
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 54. **Mohamed Taha**, M.R. Almeida, F.A. e Silva, P. Domingues, S.P.M. Ventura, J.A.P. Coutinho,* M.G. Freire, Novel Biocompatible and Self-Buffering Ionic Liquids for Biopharmaceutical Applications, *Chemistry - A European Journal* **2015**, 21, 4781–4788.
 55. B.S. Gupta, **Mohamed Taha**, M.-J. Lee.* Buffers more than Buffering Agent: Introducing A New Class of Stabilizers for the Protein BSA, *Physical Chemistry Chemical Physics* **2015**, 17, 1114–1133.
 56. P.M. Reddy, **Mohamed Taha**, Y.V.R.K. Sharma, Pannuru Venkatesu,* MingJer Lee, Quantifying the Co-Solvents Effects on Trypsin from the Digestive System of Carp Catla Catla by Biophysical techniques and molecular dynamics simulation, *RSC Advances* **2015**, 5, 43023–43035.
 57. **Mohamed Taha**, M.V. Quental, I. Correia, M.G. Freire, J.A.P. Coutinho,* Extraction and Stability of Bovine Serum Albumin (BSA) using Cholinium-Based Good's Buffers Ionic Liquids, *Process Biochemistry* **2015**, 50, 1158–1166.
 58. S. Altway, **Mohamed Taha**, M.-J. Lee,* Liquid-Liquid, Solid-Liquid, and Solid-Liquid-Liquid Equilibria of Systems Containing Cyclic Ether (Tetrahydrofuran or 1,3-Dioxolane), Water, and A Biological Buffer MOPS, *Journal of Chemical Thermodynamics* **2015**, 82, 93–98.
 59. **Mohamed Taha**, F.A. e Silva, M.V. Quental, S.P.M. Ventura, M.G. Freire, J.A.P. Coutinho*, Good's Buffers as A Basis for Developing Self-Buffering and Biocompatible Ionic Liquids for Biological Research, *Green Chemistry* **2014**, 16, 3149–3159.
 60. I. Khan, **Mohamed Taha**, P. Ribeiro-Claro, S.P. Pinho, J.A.P. Coutinho*, The Effect of the Cation on the Interactions between Alkyl Methyl Imidazolium Chloride Ionic Liquids and Water, *Journal of Physical Chemistry B* **2014**, 118, 10503–10514.
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- and Sequestration with Aqueous 2-amino-2-hydroxymethyl-1,3-propanediol (TRIS) solutions, *Journal of Physical Chemistry A* **2014**, 118, 11572–11582.
63. A. Kumar, P. Venkatesu,* **Mohamed Taha**, M.-J. Lee, Thermodynamic Contribution of Amino Acids in Ionic Liquids Towards Protein Stability, *Current Biochemical Engineering* **2014**, 1, 125–140.
 64. **Mohamed Taha**, M.-J. Lee*, TES Buffer-Induced Phase Separation of Aqueous Solutions of Several Water-Miscible Organic Solvents at 298.15 K: Phase Diagrams and Molecular Dynamic Simulations, *Journal of Chemical Physics* **2013**, 138, 244501–244514. (Selected as the cover image of this issue)
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- (O, O) Donor Ligands with Biological Relevance in Aqueous Solution. *Journal of Solution Chemistry* **2011**, 40, 1965–1986.
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77. **Mohamed Taha**, M.-J. Lee*, Solubility and Phase Separation of 4-Morpholineethanesulfonic Acid (MES) and 4-(N-Morpholino)butanesulfonic Acid (MOBS) in Aqueous 1,4-Dioxane and Ethanol Solutions, *Journal of Chemical & Engineering Data* **2011**, 56, 4436–4443.
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80. **Mohamed Taha**, M.-J. Lee*, New Insights into Buffer-Ionic Salt Interactions: Solubilities, Transfer Free Energies, and Transfer Molar Volumes of TAPS and TAPSO from Water to Aqueous Electrolyte Solutions, *Journal of Solution Chemistry* **2010**, 39, 1665–1680.
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CONFERENCES AND WORKSHOPS

1. Attendance in the Springer nature workshop entitled "Enhance your research using NANO research solution", 2018 5th Sep.
2. Active organizer in the 5th international conference on advanced sciences (ICAS5) 9-12 Nov. 2019. Hurghada, Egypt.
3. Attendance in the workshop entitled "Energy storage Devices: Challenges and Perspectives" organized on 28th September, 2020 at Faculty of Postgraduate Studies for Advanced Sciences – Beni-suef University.

4. Imran Khan, **Mohamed Taha**, Paulo Ribeiro-Claro, Simão P. Pinho, João A. P. Coutinho. The Effect of the Cation on the Interactions between Alkyl Methyl Imidazolium Chloride Ionic Liquids and Water. 9th National Conference on Thermodynamics of Chemical, Biological, Environmental and Non-Conventional Energy Systems (TCBNES-2014), 17-18 October 2014, Gujarat, India.
5. I. Khan, **Mohamed Taha**, S.P. Pinho, J.A.P. Coutinho. Study of the Interactions of Pyridinium, Pyrrolidinium or Piperidinium based Ionic liquids with Water: Infra-red Analysis and COSMO-RS Modeling. 9th National Conference on Thermodynamics of Chemical, Biological, Environmental and Non-Conventional Energy Systems (TCBNES-2014), 17-18 October 2014, Gujarat, India.
6. M.V. Quental, **Mohamed Taha**, F.A. e Silva, S.P.M. Ventura, M.G. Freire, J.A.P. Coutinho. Extraction of Bovine Serum Albumin (BSA) by Aqueous Biphasic Systems (ABS) composed of Good's buffer ionic liquids. 12th International Chemical and Biological Engineering Conference (CHEMPOR 2014), September 10-12, 2014, Porto, **Portugal**.
7. **Mohamed Taha**, F.A. e Silva, S.P.M. Ventura, F. Gonçalves, J.A.P. Coutinho, Good Buffer Ionic Liquids: A New Class of Ionic Liquids for pH Control in Aqueous and Organic Media; X CICECO Meeting; Aveiro, 2013, Portugal.
8. Dhoni Hartanto, **Mohamed Taha**, Bhupender S. Gupta, Ming-Jer Lee, Isobaric Vapor-Liquid Equilibria For The Extractive Distillation of Tert-Butanol + Water Mixtures Using Tris (Hydroxymethyl) Aminomethane at 101.3 kPa, AISC-TAIWAN 2013, Taiwan.
9. Asalil Mustain, Bhupender S. Gupta, **Mohamed Taha**, Ming-Jer Lee, New class of ionic liquids: synthesis, structural characterization and thermal properties, AISC-TAIWAN 2013, Taiwan.
10. **Mohamed Taha**, Ming-Jer Lee. Phase Behavior of Aqueous Mixtures of Tetrahydrofuran with Biological Buffer HEPES. 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Qinghai Institute of Salt Lakes, July 23-27, 2012, China.
11. Saidah Altway, **Mohamed Taha**, Ming-Jer Lee. Separation of 2-Propanol from Its Aqueous Solution with the Aid of a Biological Buffer MOPS. Symposium on Process System Engineering, May 25-26, 2012, Nantou, Taiwan.
12. **Mohamed Taha**, Ming-Jer Lee. The Effect of MES, MOPS, and MOPSO Buffers on the Conformation of the Ubiquitous "Smart" Polymer PNIPAM. International Conference on Innovation in Polymer Science and Technology, November 28-December 1, 2011, Bali, Indonesia.
13. **Mohamed Taha**, Ming-Jer Lee. Solubility and Phase Separation of MOPS and MOBS in Aqueous 1,4-Dioxane and Ethanol Solutions at 298.15 K. The 13th Asia Pacific Confederation of Chemical Engineering Congress, October 5-8, 2010, Taipei, Taiwan.

TRAINING

Employee Training

1. Digital Transformation: Fundamentals of IT; Word Processing, and Presentations, Beni-Suef University, 2022.
2. Use of Technology in Teaching, Beni-Suef University, 2021.



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3. Research Ethics, Beni-Suef University, 2021.
 4. Time and Meeting Management, Beni-Suef University, 2021.
 5. Integrity, Transparency and Anti-corruption, Beni-Suef University, 2021.
 6. Ethical Conduct and Code of Ethics, Beni-Suef University, 2021.
 7. The Credit Hour Systems, Beni-Suef University, 2017.
 8. Exams and Students Evaluation Systems, Beni-Suef University, 2017.
 9. Effective Teaching Skills, Beni-Suef University, 2017.
 10. Competing for Research Funds, Beni-Suef University, 2017.
 11. University Management, Beni-Suef University, 2017.
 12. University Code of Ethics, Beni-Suef University, 2017.