PERSONAL INFORMATION

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POSITION

Associate Professor of Physical Chemistry (Molecular Modeling and Simulations)-(7/9/2022)-Materials Science and Nanotechnology Department, Faculty of Postgraduate Studies for Advanced Sciences (PSAS), Beni-Suef University, Beni-Suef, Egypt.

Lecturer of Molecular Modeling and Simulations-(24/10/2017)-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 Science, Galala University:

1. CHE421 Molecular Modeling and simulation
2. CHE432Applications of Membrane technology & Surface Science

Faculty of Postgraduate Studies for Advanced Sciences:

1. Modelling & Simulation
2. Nanomaterials for Catalysis

3. Instrumental Analysis

Faculty of Navigation Sciences and Space Technology, Beni-Suef University.

1. Thermodynamics

Faculty of Earth Science, Beni-Suef University.

2. Thermodynamics

Sultan Qaboos University, Sultanate of Oman

3. CHEM 2101, General Chemistry I (Lab)
4. CHEM 2101, General Chemistry I (Lab)
5. CHEM 3335, Physical Chemistry I (Lab)
6. CHEM 4435, Physical Chemistry II (Lab)

WORK EXPERIENCE

[02/2017-5/2017]	Faculty visiting at Sultan Qaboos University, College of Science, Chemistry Department, Muscat, Sultanate of Oman.
[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 (113)

1. A. Abdelkarim, A.H. Zaki, S.I. El-Dek, **Mohamed Taha**. Sodium titanate ($Na_2Ti_4O_9$) nanoribbons for effective removal of organic dyes from water: Experimental and computational studies. *Journal of Molecular Liquids*, **2024**, 126414 DOI: https://doi.org/10.1016/j.molliq.2024.126414
2. E. K. Mahmoud, H.M. Mahmoud, **Mohamed Taha**. Utilizing Metal-Organic Framework Porosity for Efficient Antibiotic Separation and Sustained Release. *Surfaces and Interfaces*, **2024**, 105385. DOI: https://doi.org/10.1016/j.surfin.2024.105385
3. EK Mahmoud, SI El-Dek, AA Farghali, **Mohamed Taha**, Investigating the potential of triclinic $ABSe_3$ (A = Li, Na, K, Rb, Cs; B = Si, Ge, Sn) perovskites as a new class of lead-free photovoltaic materials, Scientific Reports 14 (**2024**), 22691
4. AM Ashraf, MH Khedr, AA Farghali, H Abdallah, **Mohamed Taha**, High-performance metal-organic frameworks for efficient adsorption, controlled release, and membrane separation of organophosphate pesticides, Journal of Environmental Chemical Engineering 12 (**2024**), 114292.
5. Elbanna, E.S., Farghali, A.A., Khedr, M.H. and **Mohamed Taha**, Nano clinoptilolite zeolite as a sustainable adsorbent for dyes Removal: Adsorption and computational mechanistic studies. Journal of Molecular Liquids, **2024**, 125538.
6. Alharbi, H.M., Eldin, Z.E., **Mohamed Taha**, M. and Elbeltagi, S. Preparation, characterization, and anticancer evaluation of polydatin conjugated with zinc MOF and encapsulated by liponiosomes as a potential nanotool-induce apoptosis. Journal of Molecular Structure, **2024**,138982.
7. **Mohamed Taha**, Essam, D., Kotp, A.A., Salah, A.M., El-Fatah, G.A., GadelHak, Y., Shehata, N., Zaher, A., Zayed, A.M., Radalla, A.M. and Mahmoud, R. Calcium ions electrochemical detection by Cu-Fe LDH/cysteine-based nanocomposite for water softening applications. Journal of Nanoparticle Research, 26, **2024**,1-16.

8. **Mohamed Taha**, Kamal, W., Essam, D., Kotp, A.A., Salah, A.M., El-Fatah, G.A., GadelHak, Y., Shehata, N., Zaher, A., Zayed, A.M. and Mahmoud, R. Co/Ni/Cu-NH2BDC MOF@ natural Egyptian zeolite ore nanocomposite for calcium ion removal in water softening applications. Environmental Science and Pollution Research, **2024**,1-17.
9. F Ayman, **Mohamed Taha**, AA Farghali, RM Abdelhamee. Synthesis and applications of porphyrin-based MOFs in removal of pesticide from wastewater: molecular simulations and experimental studies, CrystEngComm, 25, **2023**, (48), 6697–6709.
10. MHA Aouelela, **Mohamed Taha**, SI El-dek, A Hassan, AN Vasiliev, M Abdel-Hafiez, Synthesis and Characterization of Molybdenum- and Sulfur-Doped FeSe, ACS Omega, 8, **2023**, 36553–36561.
11. Asalil Mustain, Bhupender S Gupta, **Mohamed Taha**, Ming-Jer Lee. Mixtures of [TMA][EPPS] ionic liquid plus methanol, ethanol, or water: Thermophysical properties and molecular interactions. New Journal of Chemistry, 47, **2023**, 12304-12313
12. AG Zawal, MM Abdel-Aziz, AA El-Shanawani, LM Abdel-Aziz, **Mohamed Taha**, Claire Simons, SS Elbaramawi. Targeting Mycobacterium tuberculosis: Synthesis, in vitro and in silico evaluation of novel N1-(benzo[d]oxazol-2-yl)-N4-arylidine compounds. Archiv der Pharmazie, **2023**, e2300187
13. HMA Mostafa, **Mohamed Taha**, AO El-Gendy, AS Khairalla, M Abd ElFattah, M Raslan. Antimicrobial and antivirulence saponins of Mimusops laurifolia leaves. Letters in Applied Microbiology, 76, **2023**, ovad071
14. A Belal, R Mahmoud, **Mohamed Taha**, FM Halfaya, A Hassaballa, ES Elbanna, E Khaled, A Farghali, FI Abo El-Ela, SM Mahgoub, MM Ghoneim, MY Zaky. Therapeutic Potential of Zeolites/Vitamin B12 Nanocomposite on Complete Freund's Adjuvant-Induced Arthritis as a Bone Disorder: In Vivo Study and Bio-Molecular Investigations. Pharmaceuticals, **2023**, 16(2), 285
15. A Belal, R. Mahmoud, EE Mohamed, A Farghali, FI Abo El-Ela, A Gamal, FM Halfaya, E Khaled, AA Farahat, AHE Hassan, MM Ghoneim, **Mohamed Taha**, MY Zaky. A Novel Hydroxyapatite/Vitamin B12 Nanoformula for Treatment of Bone Damage: Preparation, Characterization, and Anti-Arthritic, Anti-Inflammatory, and Antioxidant Activities in Chemically Induced Arthritic Rats. Pharmaceuticals, **2023**, 16(4), 551
16. 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
17. **Mohamed Taha**, RA Abdelhay, MH Khedr. Vacancy defects transform zinc tellurite glass from insulator to semiconductor: A first-principles prediction. Optik, **2022**, 271, 170125
18. EK Mahmoud, AA Farghali, SI El-dek, **Mohamed Taha**. Structural stabilities, mechanical and thermodynamic properties of chalcogenide perovskite ABS3 (A= Li, Na, K, Rb, Cs; B= Si, Ge, Sn) from first-principles study. European Physical Journal Plus, **2022**, 137(9), 1006.
19. HH AbdElAziz, **Mohamed Taha**, WMA El Rouby, MH Khedr, L Saad. Evaluating the performance of Cs2PtI6−xBrx for photovoltaic and photocatalytic applications using first-principles study and SCAPS-1D simulation. Heliyon, **2022**, 8(10), e10808

20. 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
21. 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
22. HE Emam, M El-Shahat, **Mohamed Taha**, RM Abdelhameed. Microwave assisted post-synthetic modification of IRMOF-3 and MIL-68-NH_2 onto cotton for Fuel purification with computational explanation. Surfaces and Interfaces, **2022**, 30, 101940
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27. 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.
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36. 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.
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39. 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.
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45. A. Abdel-Moneim,* A.A.G. El-Shahawy, A.I. Yousef, S.N. Abd El-Twab, Z.E. Elden, **Mohamed**

Taha, Novel polydatin-loaded chitosan nanoparticles for safe and efficient type 2 diabetes therapy: in silico, in vitro and in vivo approaches, *International Journal of Biological Macromolecules* **2020**, 154, 1496-1504.

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47. H.R.Abd El-Mageed and **Mohamed Taha**,* Exploring the intermolecular interaction of serine and threonine dipeptides with gold nanoclusters and nanoparticles of different shapes and sizes by quantum mechanics and molecular simulations, *Journal of Molecular Liquids* **2019**, 296, 111903.

48. 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.

49. H.A. Younes, R.K. Mahmoud,* H.M. Mahmoud, H.F. Nassar, M.M. Abdelrahman, F.I. Abo El-Ela, **Mohamed Taha**, Computational and experimental studies on the efficient removal of diclofenac from water using ZnFe-layered double hydroxide as an environmentally benign absorbent, *Journal of the Taiwan Institute of Chemical Engineers* **2019**, 102, 297-311.

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52. 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.

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54. 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.

55. **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.

56. 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.

57. 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.

58. 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.
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60. **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.
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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 worshop entitled “Energy storage Devies: Challenges and Perspectives” organized on 28th September, 2020 at Faulty of Postgraduate Studies for Advaned Scienes – Beni-suef Univeristy.
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 Distilation 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. 15thInternational Symposium on Soluility 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.
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.