

Ain Shams University  
University College of Women  
(Arts, Science and Education)  
Physics department



جامعة عين شمس  
كلية البنات للاداب والعلوم و التربية  
قسم الفيزياء

## CV

- Full name** Hanan Gouda AbdElwahab Ahmed ElHaes
- Date of birth** 23-2-1970, Elkalyoubia, Egypt.
- Nationality** Egyptian
- Marital Status** Married and has three daughters
- Address** 31 El Ansar Str.- ElDokky  
Giza - Egypt.  
Tel.: 00202-37627538  
Mob.: 002-01011847432
- e-mail**  
[medahmed@yahoo.com](mailto:medahmed@yahoo.com)  
[hanan.elhaes@women.asu.edu.eg](mailto:hanan.elhaes@women.asu.edu.eg)
- Educational Background:**
- B.Sc. in Physics, Faculty of Women for Arts, Science, and Education, AinShamsUniversity, **May 1992**
  - M.Sc. in Experimental Physics, Faculty of Women for Arts, Science, and Education, AinShamsUniversity, **April 1998**  
Entitled:  
*'Effect of spray parameters on some physical and spectral properties of Iron Oxide thin film '*
  - Ph.D. in Experimental Physics, Faculty of Natural Science, Information and Mathematics, RWTH-Aachen University, Germany.  
Entitled:  
*"Magnon heat transport and magnon-hole scattering in one and two dimensions spin systems"*
- Position**
- May 1992 to April 1998**, Demonstratorat Faculty of Women for Arts, Science, and Education, AinShamsUniversity
  - April 1998 to July 1999**, Assistant Lecturer at Faculty of Women for Arts, Science, and Education, AinShamsUniversity - Egypt
  - July 1999 to October 2004**, granted a Scholarship for Ph.D. study in Germany.
  - December 2004 up till 27-3-2010**, Lecturer at Faculty of Women for Arts, Science, and Education, AinShamsUniversity.
  - 17-10-2008** Assistant Professor, Faculty of Science for Girls-JazanUniversity.



**17-4-2009 up till 25-6-2011**, Head of Physics department, Faculty of Science for Girls-Jazan University.

**27-3-2010 up 29-9-2015**, Associate professor at Faculty of Women for Arts, Science, and Education, Ain Shams University.

**29-9-2015 up till now**, professor at Faculty of Women for Arts, Science, and Education, Ain Shams University.

**23-8-2016 up 23-8-2019**, Head of Physics department, Faculty of Women for Arts, Science, and Education, Ain Shams University.

**16-17 January 2012** Egyptian-Italian Science Forum 2012, Rome, Italy.

**28 January 2014 to 07 February 2014** Visiting Professor, CNR, Research Area 1, Rome, Italy

**18 September 2016 to 30 September 2016** Visiting Professor, CNR, Research Area 1, Rome, Italy.

**31 January 2017 to 10 February 2017** Visiting Professor, CNR, Research Area 1, Rome, Italy.

**01 July 2018 to 30 July 2018** Visiting Professor, Department of Neutron Activation Analysis and Applied Research, Division of Nuclear Physics, Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia.

**6/2020 till 9/2021** Director of E-Learning unit, Faculty of Women for Arts, Science, and Education.

**Papers: 126 international papers: list attached.**

**H- index: 20**

**Total citation: 1623**

#### **International talks and Conferences**

1. P. Reutler, R. Kessler, J. Geckl, D. Bruns, R. Klingeler, **H. ElHaes**, B. Buechner and A. Revcolevschi, 2002 "Ladungsordnung in  $(La_{1-y}Pry)_7/8Sr_{1/8}MnO_3$  Manganaten" Deutsche Physikalische Gesellschaft e. V. (DPG)E-Verhandlungen 2002, Regensburg (11. - 15. März 2002).
2. C. Hess, U. Ammerahl, C. Baumann, D. Bruns, D. Cassel, L. Colonescu, O. Friedt, **H. ElHaes**, M. Hücker, B. Büchner, M. Braden, A. Revcolevschi, S-W. Cheong, F. Heidrich-Meisner and W. Brenig, 2002 "Thermal Transport in Transition Metal Oxides with Low-Dimensional Structures of Charge and Spin" Ladungsordnung in  $(La_{1-y}Pry)_7/8Sr_{1/8}MnO_3$  Manganaten", Deutsche Physikalische Gesellschaft e. V. (DPG), E-Verhandlungen 2002, Regensburg (11. - 15. März 2002).
3. **H. ElHaes**, C. Hess, B. Buechner, M. Huecker, U. Ammerahl and A. Revcolevschi, 2003 "Magnon-Hole Scattering in  $Sr_{14-x}Ca_xCu_{24}O_{41}$ " Deutsche Physikalische Gesellschaft e. V. (DPG), E-Verhandlungen 2003, Dresden (24. - 28. März 2003).



Physics Department

4. P. Ribeiro, P. Reutler, C. Hess, **H. ELHaes**, B.Buechner, G. Roth, and S. Richter, 2003 "Niedrigdimensionale Kuprate: Kristallzüchtung und Wärmeleitfähigkeit", Deutsche Physikalische Gesellschaft e. V. (DPG), E-Verhandlungen 2003, Dresden (24. - 28. März 2003).
5. **H. ELHaes**, C. Hess, P. Ribeiro, B. Buechner, M. Huecker, U. Ammerahl, A. Revcolevschi, F. Heidrich-Meisner and W. Brenig 2004 "Magnon heat transport of 2-leg spin ladders: Scattering on holes and static defects" Deutsche Physikalische Gesellschaft e. V. (DPG), E-Verhandlungen 2004, Regensburg (08.-12.03.2004).
6. C. Hess, **H. ELHaes**, P. Ribeiro, B. Buechner, F. Heidrich-Meisner, W. Brenig, M. Huecker, U. Ammerahl und A. Revcolevschi 2004, "Heat Transport in Low Dimensional Spin Systems" Deutsche Physikalische Gesellschaft e. V. (DPG), E-Verhandlungen 2004, Regensburg (08.-12.03.2004).
7. G. M. El Komy, **H. ELhaes**, M. Ibrahim, J. Liu, J. Huang, M. Selim, "Sensor Technology and Nano Devices of Tin Oxide Films Prepared by Sol Gel", The International Conference For Nanotechnology Industries The Leading Technology of 21st Century" Riyadh, Saudi Arabia, 5-7 April, 2009.
8. **Hanan Elhaes**, Abdullah Al-Hossain, Afaf Babaier and Medhat Ibrahim, "Spectroscopic Analysis of Fullerene Alkali Dimer, The 2nd International Conference on Advanced Materials and their Applications and its workshop on "New Trends in Nano-science and laser Physics" Cairo, Egypt, 6-8 April 2010
9. **Hanan Elhaes**, Hanan Moawad, and Medhat Ibrahim "Computational Analyses of the Chromium Interaction with Protein" 1st International Conference on Electrical and Computer Systems Engineering (ECSE 2010), Cairo, Egypt, **November 1-3, 2010**
10. Osama Osman, Medhat Ibrahim, and **Hanan Elhaes** "Interaction of Nano Structure Material with Heme Molecule: Modelling Approach" 1st International Conference on Electrical and Computer Systems Engineering (ECSE 2010), Cairo, Egypt, November 1-3, 2010.
11. Medhat Ibrahim and **Hanan Elhaes**, "Exploring Materials Using Molecular Modeling", Egyptian-Italian Science Forum 2012, Rome, Italy, January 16-17, 2012 (Talk).
12. Abd el baset H. Makky, **Hanan Elhaes**, Mohamed M. El-Oker and Medhat A. Ibrahim "Synthesis, Electronic Properties of some Fullerene Based Systems" International Conference on Material Science and Applications (ICMSA 2012), Taif University, Saudi Arabia, 2012.
13. **Hanan Elhaes**, Medhat Ibrahim, Gusabina Cabriouty "Effect of Salinity on the Molecular Structure of Soil of Archaeological Sites: Spectroscopic and Modelling Approach", the 5th National Conference on Optical Spectroscopy, Laser and their Applications 24 - 27 March 2014. NRC, Cairo, Egypt.
14. Mohamed Morsy, **Hanan Elhaes**, Medhat Ibrahim, "High Purity Multi-Wall Carbon Nano Tube for Environmental Applications", 2nd International Conference on "Biotechnology and Environmental Safety" May 6-8, 2014.
15. Medhat Ibrahim, Hanan Ibrahim and **Hanan Elhaes**, "Modeling and Spectroscopic Analyses of Water Hyacinth", The 23rd International Conference on High Resolution Molecular Spectroscopy, Bolonga, Italy September, 2-6, 2014.
16. Medhat Ibrahim, and **Hanan Elhaes** "Preservation of Stone-Based Monuments: Molecular Modeling Approach", the 3rd International Conference on Advanced Materials and Their Applications, National Research Centre, Egypt, January 11-13, 2015.
17. Osama Osman and **Hanan Elhaes** "Interaction of Nano Metal Oxide with Heme Molecule", the 6th International Conference on Optical Spectroscopy, Laser and their Applications 7 -9 April 2015. NRC, Cairo, Egypt.



- 18 Medhat Ibrahim , Osama Osman, Abdel Aziz Mahmoud and **Hanan Elhaes**, "Towered the Nature: Nano Modified Microsphere For Remediation of Heavy Metals", the 32<sup>nd</sup> Eg-MRS International Conference, 6<sup>th</sup> -9<sup>th</sup> Jan 2016, Aswan, Egypt
- 19 Dina Ezzat, Abdel Aziz Mahmoud, Mahmoud El-Nahas and **Hanan Elhaes**" AC Conductivity and Dielectric Properties of ZnO/Cellulose Acetate Blend", the 7<sup>th</sup> International Conference on Optical Spectroscopy, Laser and their Applications 18 -20 October 2016. NRC, Cairo, Egypt.
- 20 Aly Okasha, Fathia Gomaa, **Hanan Elhaes**, Mohamed Morsy , Sherif El-Khodary, Ahmed Fakhry, Medhat Ibrahim, 2017 "Spectroscopic analyses of the photocatalytic behavior of nano titanium dioxide", The 3<sup>rd</sup> International Conference on "Biotechnology and Environmental Safety" , NRC, Cairo, 14-16 March, 2017.
- 21 **Hanan Elhaes** and Medhat Ibrahim 2017 "Spectroscopic Analyses for the Effect of Salinity on Soil", The 3<sup>rd</sup> International Conference on "Biotechnology and Environmental Safety" , NRC, Cairo, 14-16 March, 2017.
- 22 Medhat Ibrahim and **Hanan Elhaes** 2017 " Theory and Molecular Modeling: Applied to Nanoscience", The 9<sup>th</sup> International Conference on Nano Technology in Construction (NTC 2016) 17-21 March 2017, Sharm El-Sheikh-Egypt.
- 23 **Medhat Ibrahim** and Hanan Elhaes 2017 :Molecular Modeling As a Tool for Analyses and Assignments of Polymers", 13<sup>th</sup> Arab International Conference on Polymer Science and Technology 22-25 October 2017, Sharm El-Sheikh-Egypt.
- 24 **Hanan Elhaes**, Ahmed Refaat and Medhat A. Ibrahim " Molecular Modeling Analyses for Metal Oxide/Graphene" Egypt-Japan University of Science and Technology, New Borg El-Arab, Alexandria, Egypt, 11-13 March 2018
- 25 **H. Elhaes**<sup>1</sup>, A. Refaat and M. A. Ibrahim, Effect of CaO, MgO and SrO on the physical properties of graphene. 10<sup>th</sup> International Conference on NANO-TECHNOLOGY IN CONSTRUCTION (NTC 2018) 13-17 April 2018, Hurgada, Egypt
- 26 **Hanan Elhaes**, Modeling the Effect of Metal Substitution on the Electronic Properties of Fullerene and Fullerypyrrolidine, The First International Conference on Molecular Modeling and Spectroscopy, National Research Centre, Cairo, Egypt, 19-22 February 2019.
- 27 Rania badry, **Hanan Elhaes** and Medhat Ibrahim , Polyaniline Substituted with Alkali and Alkaline Earth Elements: Molecular Modeling Approach 11<sup>th</sup> International Conference on NANO-TECHNOLOGY IN CONSTRUCTION (GREEN AND SUSTAINABLE CONSTRUCTION) (NTC 2019), 22-26 March 2019, Sharm El-Sheikh-Egypt

#### Attend the following conferences and seminars

**Conference:** Fourth National Conference, Science and environment, Al-Azhar University., Cairo, 17 – 19 Sept., 1999.

**Conference:** First International conference on Advanced Materials and Their applications, 12-14 December, 2005. NationalResearchCenter, Cairo, Egypt

NorbertKreidlMemorialinternational course and Conference on Science and Technology of Advanced Glasses, Building Bridges Between Glass Science and Technology and Between Cultures, AUC, Cairo, Egypt 2006.



**Seminar:** Application of Spectroscopy in Medicine, Industry and Environment, (Spectroscopy Department Annual Seminar- 2006)

**Workshop:** Biological and Industrial Applications of Gas Sensors, NRC, Cairo 17-01-2008, Egypt-China agreement.

**Seminar:** Physics in Our Life, NRC, Cairo 30-04-2012.

**Workshop:** Application of Molecular Modeling, NRC, June 24-25, 2013.

**Seminar:** One Day Seminar: Raman Technologies: An Overview, NRC, September 25, 2013.

**Workshop:** Technologies for the Egyptian Cultural Heritage (TECH) Workshop in the framework of the Agreement of ASRT, Egypt & CNR, Italy. CNR, Rome, Italy, February 0, 2014.

**Conference:** 5th National Conference on Optical Spectroscopy, Laser and their Applications 24 - 27 March 2014. NRC, Cairo, Egypt.

**Conference:** The 2<sup>nd</sup> International Conference on "Biotechnology and Environmental Safety" NRC, May 6-8, 2014.

**Seminar:** Modern Applications in Physics, National Research Center, Cairo, Egypt, April 9, 2014.

**Workshop:** Molecular Modeling: Theory and Applications, NRC, June 17, 2014.

**Conference:** The 23rd International Conference on High Resolution Molecular Spectroscopy Bologna, Italy, September 2-6, 2014.

**Seminar:** Solar Energy: Materials, Applications and Challenges, NRC, Cairo, Egypt, October 14, 2014.

### **Seminars, Workshops and Conferences (as organizer)**

**Workshop:** Coordinator of the First Workshop: **Applications of Molecular Modeling**, Physics Department, Faculty of Women for Arts, Science and Education, Ain Shams University, Cairo, Egypt, April 25-26, 2017.

**Workshop:** Coordinator of the Second Workshop: **Estimation of HOMO/UMO Band Gap Energy**, , Physics Department, Faculty of Women for Arts, Science and Education, Ain Shams University, Cairo, Egypt, September 19-20, 2018.

**Workshop:** Coordinator of the Workshop "**Modeling and Simulation** at Molecular Modeling Clube, El-Manshya, Qalyobia, 02-05 October 2018.

**Winter School:** Coordinator of the **First Spectroscopy Winter School SWS-1**, Physics Department, Faculty of Women for Arts, Science and Education, Ain Shams University, Cairo, Egypt, 12-16 December 2018.

**Conference:** Coordinator of the First International Conference on Molecular Modeling and Spectroscopy, National Research Centre, Cairo, Egypt, 19-22 February 2019.

**Winter School:** The Second Spectroscopy Winter School SWS-2, Ismaillia, Egypt, 25-31 January 2020.

**Online Conference:** The second international conference on molecular modeling and spectroscopy, September 23-24, 2020

**Winter School:** The Third Spectroscopy Winter School SWS-3, Cairo, Egypt, 25-31 February 2021.

**Online Conference:** The Third International Conference on Molecular Modeling and Spectroscopy, September 15-16, 2021



## Supervision

### Finished Thesis

1. Abdel Baset Hofny, "Electronic Properties of some Fullerene Based Systems", Physics Department, Al-Azhar University. PhD.
2. Mohamed Attallah, "Optical and Physical behavior of glasses doped with some transition metal elements", Physics Department, Al-Azhar University. PhD.
3. Dina Ezzat, "Some Physical and Spectral Analyses of Cellulose Derivatives", Physics Department, Ain Shams University. MsC.
4. Rania Badry, Preparation and Characterization of Some Polymer Blend, MsC
5. Dina Ezzat, Some Physical Characteristic of Cellulose Acetate Doped with Different Nano Metal Oxides and its Applications, PhD

### Running Thesis

1. Rania Badry, Spectroscopic Study for Nano-Composites of Natural Polymer and Nano Metal Oxides, PhD

### Prizes and Awards

#### 1- Prof. Dr. Mohamed Ameen Lotfy Prize for Physical Sciences, 2011.

1. **HananElhaes**, Medhat Ibrahim, Mahmoud Sleim, Jinhuai Liu, and Jiarui Huang, 2009 "SnO<sub>2</sub> as a Gas Sensor: Modeling and Spectroscopic Approach" SENSOR LETTERS, Vol. 7, 530–534.
2. **HananElhaes**, AfafBabaer and Medhat Ibrahim, 2010 "Effect of Metal Substitution on the Electronic Properties of Fullerene and Fullero pyrrolidine" J. Comput. Theor. Nanosci. 7, 536-541...
3. Abo-el-nour N. Abd-alla, Hassan a. Eshaq and **HananElhaes**, 2011 "The phenomena of reflection and transmission waves in smart nano materials", J. Comput. Theor. Nanosci. , 8, 1670–1678.
4. **HananElhaes** and Afaf Babaier, 2011 "Studying the Electronic Properties of Fullerene Alkali Dimers", J. Comput. Theor. Nanosci. , 8, 1509-1512.

## Projects

1. **Molecular Modeling and Experimental Neutron Scattering Studies of Interactions of the Condensed Matter and Biological (Lipid Membranes) Systems. ASRT- JINR bilateral project**

**Duration: 01-07-2020 to 30-07- 2022.**

2. **Molecular Modeling Analyses of the Effect of Nano Metal Oxides on Biological Molecules. (Member): ASRT- JINR bilateral project.**

**Duration: 01-12-2018 to 30-11-2019**

3. **Spectroscopic analyses for natural microsphere for maximizing its application in the remediation of inorganic pollutants. : NRC-CNR agreement: ID: IT1022**

**Duration: 20-03-2016 to 19-03-2018.**

4. **Cost Effective Design and Implementation of Microsphere production for Wastewater Treatment (Member I): ASRT-1217 ASRT Initiative**

**Duration: 24-12-2016 to 23-12-2018.**

5. **Molecular Modeling Applications of Some Bio-Polymers - PI: STDF 14990**

**Duration: 8-12-2015 to 7-12-2017.**



6. Spectroscopic analyses of some fullerene-based systems containing dithiocarbamate moieties (Co-PI): STDF 4347

**Duration:** 17-06-2012 to 16-12-2015.

7. On the Structural Analyses of Multifunctional Natural Microsphere. (Co-PI): STDF 4371

**Duration:** 18-3-2014 to 17-3-2016.

8. Photogrammetry: Technology for the Egyptian Cultural Heritage (TECH) ASRT-NCR Agreement.

**Duration:** 24-12-2013 to 23-12-2015.

9. Effect of Salinity on the Molecular Structure of Jazan Soil. (Member): Jazan University, KSA., 029/ 1434 H

**Duration:** 02-04-2012 to 01-04-2013.

10. Reflection and Refraction of Waves in Nano-Smart Materials (Anisotropic Thermo-piezoelectric Materials). (Member): Jazan University, KSA., 020/ 1431 H

**Duration:** 02-04-2012 to 01-04-2013

11. Development of Natural Blends for Removal of Organic Pollutants. (Member): Taif University, KSA. 1-143-1975.

**Duration:** 23-01-2012 to 22-01-2013.

12. Member in the project of scientific cooperation between Egypt and China entitled: Preparation of gas sensors based on Carbon Nanotube / thin film of semiconductor oxide and its application.

**Duration:** 01-01-2007 to 30-12-2010.

13. Molecular Modeling Approach for the Design and Evaluation of Hepatitis C Virus Inhibitors. Funded by Cairo University.

**Duration:** 01-07-2011 to 30-06-2012.

1. Member of the Egyptian Materials Research Society.
2. Member of the Egyptian Crystallography Society.
3. Member of the German Society of Physics (DPG).
4. Member of the Egyptian Syndicate of Scientific Missions.
5. National Committee for Women in Science 2018 to 2021.
6. International Society of Muslim Women in Science, USA
7. National Committee for Crystallography 2022



## List of Publications

<b>Full name</b>	Hanan Gouda AbdElwahab Ahmed Elhaes
<b>List of Publications</b>	
<b>2022</b>	
<b>Published</b>	
<b>2021</b>	
1.	Hegazy M.A.Ghoneim R.,Ezzat H.A.,Yahia I.S., Elhaes H.,Ibrahim M. A., “Electronic and physical studies for Teflon FEP as a thermal control in low earth orbit reinforced with ZnO and SiO <sub>2</sub> nanoparticles” Journal of Molecular Modeling, 2021, 27(10), 295
2.	Ezzat, D., Youssif, M., <b>Elhaes, H.</b> , El-Nahass, M. Dielectric relaxation behaviour and ac electrical conductivity of cellulose acetate-molybdenum trioxide nanoparticle blended film Egyptian Journal of Chemistry, 2021, 64(3), pp. 1125–1132
3.	<b>H. Elhaes</b> , M. Morsy, I. S. Yahia and M. Ibrahim, “Molecular modeling analyses for electronic properties of CNT/TiO <sub>2</sub> nanocomposites”, Optical and Quantum Electronics. 53(5), (2 May 2021)269.
4.	Ahmed Fahmy, Rasha M. Khafagy, <b>Hanan Elhaes</b> , Medhat A. Ibrahim, Molecular Modeling Analyses of Polyvinyl Alcohol/ Sodium Alginate/ZnO Composite, Egypt. J. Chem. 64 (3), (2021) 1149-1166.
5.	Taha M.Tiama, <b>Hanan Elhaes</b> , Medhat A. Ibrahim,” Application of Chitosan/Fe <sub>3</sub> O <sub>4</sub> Nanocomposite as Biosensor”, Letters in Applied NanoBioScience, 10 (3), (2021), 2438-2445
6.	Ahmed M. Bayoumy, Yasmine O. Osman, <b>Hanan Elhaes</b> , Medhat A. Ibrahim, Mohamed A.M. El-Mansy "Effect of Substitutions on the Electronic Properties of Acetylsalicylic Acid", Optical and Quantum Electronics. 53(1), (2021) 59.
7.	Rania Badry, Ahmed Fahmy, Asmaa Ibrahim, <b>Hanan Elhaes</b> and Medhat Ibrahim,"Application of Polyvinyl alcohol/Polypropylene/Zinc Oxide Nanocomposites as Sensor: Modeling Approach", Optical and Quantum Electronics. 53(1) (2021) 39
8.	Hend Ezzat, <b>Hanan Elhaes</b> , Ahmed Refaat, Mohamed S. Abdel-Aal and Medhat A. Ibrahim, Molecular Modeling Analyses and Vibrational Characteristics for Nitromethane, Egypt. J. Chem. 64, (1), (2021) 75-84.
9.	Amina Omar, Hend Ezzat, <b>Hanan Elhaes</b> , Medhat A. Ibrahim,” Molecular Modeling Analyses for Modified Biopolymers”, Biointerface Research in Applied Chemistry, 11(1), 2021, 7847-7859
10.	Rania Badry, Hend A. Ezzat, Sherif El-Khodary, Mohamed Morsy, <b>Hanan Elhaes</b> , Nadra Nada and Medhat Ibrahim, Spectroscopic and Thermal Analyses for the Effect of Acetic Acid on the Plasticized Sodium Carboxymethyl Cellulose, Journal of Molecular Structure, 1224 (15





January, 2021) , 129013

11. Mohamed A. M. El-Mansy, Ahmed Bayoumy, Hend Ezzat, Nayera El-Sayed, **Hanan Elhaes**, Osama Osman, Abdel Aziz Mahmoud, and Medhat Ibrahim, "Modeling the Effect of Hydration on the Electronic and Vibrational Properties of AZT", *Biointerface Research in Applied Chemistry*, 11 (2), (2021), 9253 – 9265.
12. Rania Badry, Sherif El-Khodary, **Hanan Elhaes**, Nadra Nada and Medhat Ibrahim, "Optical, Conductivity and Dielectric Properties of Plasticized Solid polymer Electrolytes Based on Blends of Carboxymethyl Cellulose Sodium and Polyethylene Oxide", *Optical and Quantum Electronics*. 53 (3) (2021) 1-15
13. Rania Badry, **Hanan Elhaes**, Nadra Nada and Medhat Ibrahim" Study of the Electronic Properties of Solid Polymer Electrolytes based on blends of CMC, PEO and acetic acid", *Biointerface Research in Applied Chemistry*. 11(3), (2021), 11009-11022.
14. Ahmed Abdel Moez, Ahmed Fahmy, Hend Ezzat, Asmaa M. Ibrahim, Dina Shehata, **Hanan Elhaes**, Medhat A. Ibrahim," Molecular Modeling Analyses for Polypropylene/Zinc Oxide Nanocomposite", *Biointerface Research in Applied Chemistry*. 11 (4), (2021), 11347-11356.
15. Ahmed M. Bayoumy, Islam Gomaa, **Hanan Elhaes**, Mohamed Sleim, Medhat A. Ibrahim, Application of Graphene/Nickel Oxide Composite as a Humidity Sensor, *Egypt. J. Chem.*64, (1), (2021) 85-91.
16. Hend Ezzat, **Hanan Elhaes**, Ahmed Refaat, Mohamed S. Abdel-Aal and Medhat A. Ibrahim, Molecular Modeling Analyses and Vibrational Characteristics for Nitromethane, *Egypt. J. Chem.* 64, (1), (2021) 75-84.

### 2020

17. Rania Badry, Asmaa Ibrahim, Fatma Gamal, Samah A. Ibrahim, Hend Ezzat, **Hanan Elhaes**, Medhat Ibrahim, "Modeling the Effect of Zinc Oxide on the Electronic Properties of Polyvinyl Alcohol", *Egypt. J. Chem.*
18. H. A. Ezzat, M. A. Ibrahim and **H. El-Haes**, "Molecular Modeling Applied For Carbon Nano Materials", *Egypt. J. Chem.* Vol. 63, No. 12 pp. 4777 - 4787 (2020)
19. Hend A. Ezzat, Islam Gomaa, Alaa El-Din A. Gawad, Osama Osman, Abdel Aziz Mahmoud, Mohamed S. Abdel-Aal, **Hanan Elhaes** and Medhat A. Ibrahim, Semiempirical Molecular Modeling Analyses for Graphene/Nickel Oxide Nanocomposite. *Letters in Applied NanoBioScience*, 9(4), (2020), 1459 - 1466
20. FanliMeng, Xinyou Meng, Yuanlong Chang, Zhenyu Yuan, Hua Zhang, Medhat Ibrahim, **Hanan Elhaes** and Ibrahim Yahia, HongliangGao, Nanocomposites of ZnO Nanorods In- Situ Grown on Graphitic Carbon Nitride for Ethanol Sensing, *IEEE Sensors Journal*, 20(4), 8880691, pp. 1721-1729
21. Mohamed A. M. El-Mansy Osama Osman, Abdel Aziz Mahmoud, **Hanan Elhaes**, Alaa El-Din A. Gawad and Medhat Ibrahim, "Computational Notes on the Chemical Stability of Flutamide", *Letters in Applied NanoBioScience*. 9 (3), 2020, 1147-1155.
22. RaniaBadry, Sara H. Radwan, Dina Ezzat, Hend Ezzat, **Hanan Elhaes**, Medhat Ibrahim, "Study of the Electronic Properties of Graphene Oxide/(PANi/Teflon)", *Biointerface Research in Applied Chemistry*. Volume 10, Issue 6, 2020, 6926 - 6935
23. Medhtat A. Ibrahim, Hend A. Ezzat, Fanli Meng, Ibrahim S. Yahia, HebaY. Zahran and **HananElhaes**, " Computational Notes on The Effect of (Li-Na-K) on Calcium Zinc Phosphate Oxide Glasses", *Biointerface Research in Applied Chemistry*. Volume 10, Issue 6, 2020, 6906 - 6911
24. Mohamed A. M. El-Mansy Osama Osman, Abdel Aziz Mahmoud, **Hanan Elhaes** and Medhat



- Ibrahim, "Computational Notes on the Molecular Modeling Analyses of Flutamide", Letters in Applied NanoBioScience. 9 (2), 2020, 1099-1102.
25. Asmaa Ibrahim, **Hanan Elhaes** and Medhat Ibrahim, "Computational Notes on the Electronic Properties of Carboxylic Acid", Letters in Applied NanoBioScience. 9 (2), 2020, 1079-1082.
26. Rania Badry, Asmaa Ibrahim, Fatma Gamal, Dina Shehata, Hend Ezzat, **Hanan Elhaes** and Medhat Ibrahim, "Electronic Properties of Polyvinyl Alcohol/TiO<sub>2</sub>/SiO<sub>2</sub> Nanocomposites", Biointerface Research in Applied Chemistry. 10(5), 2020, 6427- 6435.
27. Ahmed Abdel-Karim, **Hanan Elhaes**; Amer S El-Kalliny; Mohamed I Badawy; Medhat Ibrahim; Tarek A Gad-Allah, " Probing Protein rejection behavior of blended PES-based flat-sheet ultrafiltration membranes: A density functional theory (DFT) study", Spectrochimica Acta A. 238 (2020) 118399
28. Ahmed Refaat, **Hanan Elhaes**, Nabila S. Ammar, Hanan S. Ibrahim and Medhat Ibrahim, "Green Route for the Removal of Pb from Aquatic Environment", Combinatorial Chemistry & High Throughput Screening. (2020) 23: 1.  
doi.org/10.2174/1386207323666200127123349.
29. Ahmed M. Bayoumy, **Hanan Elhaes**, Osama Osman, Tarek Hussein and Medhat A. Ibrahim, "Mapping Molecular Electrostatic Potential for Heme Interacting with Nano Metal Oxides", Biointerface Research in Applied Chemistry. 10 (2), 2020, 5091 – 5095
30. Ahmed M. Bayoumy, **Hanan Elhaes**, Osama Osman, Kholmurzo T. Kholmurodov, Tarek Hussein and Medhat A. Ibrahim, "Effect of Nano Metal Oxides on Heme Molecule: Molecular and Bimolecular Approaches", Biointerface Research in Applied Chemistry. 10 (1), 2020, 4837-4845.
31. Ahmed M. Bayoumy, Ahmed Refaat, Ibrahim S. Yahia, Heba Y. Zahran, **Hanan Elhaes**, Medhat A. Ibrahim and Mohd. Shkir, "Functionalization of Graphene Quantum Dots (GQDs) with Chitosan Biopolymer for Biophysical Applications", Optical and Quantum Electronics, 52, 2020, 16
32. Ahmed Fahmy, Rasha M. Khafagy, **Hanan Elhaes** and Medhat A. Ibrahim, "Molecular Properties of Polyvinyl Alcohol/Sodium Alginate Composite", Biointerface Research in Applied Chemistry. 10 (1), 2020, 4734-4739.
- 2019**
33. Ahmed Refaat, Daaa Atta, Osama Osman, Abdel Aziz Mahmoud, Sherif El-Kohadary, Wadea Malek, Marco Ferretti, **Hanan Elhaes** and Medhat Ibrahim, "Analytical and Computational Study of Three Coptic Icons in Saint Mercurius Monastery, Egypt", Biointerface Research in Applied Chemistry. 9 (6), 2019, 4685-4698.
34. Ahmed M. Bayoumy, Rania Badry, Heba A. Gaber, Sarah A. Elbiomy, Shima G. El Gabaly, Mariam Sayed Abd ElAziz, Shrouk Mohamed Gouda, **Hanan Elhaes**, Ibrahim S. Yahia, H.Y. Zahran and Medhat Ibrahim, "Molecular modeling analyses for the effect of solvents on amino acids", Biointerface Research in Applied Chemistry. 9(5), (2019), 4379-4383.
35. Gharieb W Ali, Wafa I. Abdel-Fattah, **Hanan Elhaes**, Medhat A. Ibrahim, "Spectroscopic and modeling analyses of bimolecular structure of corn silk", Biointerface Research in Applied Chemistry. 9 (6), 2019, 4481-4485.
36. H. Ezzat, R. Badry, I.S. Yahia, H.Y. Zahran, A. Ibrahim, **H. Elhaes** and M.A. Ibrahim, "Mapping the molecular electrostatic potential of fullerene", Egypt. J. Chem. 6 (2019) 1391-1402.
37. Asmaa Ibrahim, Hanan Elhaes, Fanli Meng and Medhat Ibrahim, "Effect of Hydration on the Physical Properties of Glucose", Biointerface Research in Applied Chemistry. 8 (4), 2019, 4114-4118.



38. Shimaa G. El Gabaly, Gehan M. Youssif, Ahmed M. Bayoumy, Hend Ezzat, **Hanan Elhaes**, Ahmed Refaat and Medhat A. Ibrahim,” Modeling The Effect of Functional Groups on The Electronic Properties of Benzene, Pyridine and Pyrimidine”, Egypt. J. Chem. Special issue, the First International Conference on Molecular Modeling and Spectroscopy, 7-(2019) 1-11
39. Dilshod D. Nematov, Amondullo S. Burhonzoda, Mirzoaziz A. Khusenov, Kholmirzo T. Kholmurodov, **Hanan Elhaes** and Medhat A. Ibrahim, “ The Quantum-Chemistry Calculations of Electronic Structure of Boron Nitride Nanocrystals with Density Functional Theory Realization”, Egypt. J. Chem. Special issue, the First International Conference on Molecular Modeling and Spectroscopy,7, (2019) 21-27
40. R. Badry, S. El-Kohdary, **Hanan Elhaes** and N. Nada and Medhat A. Ibrahim, “The Influence of Moisture on the Electronic Properties of Monomer, Dimer, Trimer and Emeraldine Base Sodium Carboxymethyl Cellulose”, Egypt. J. Chem. Special issue, the First International Conference on Molecular Modeling and Spectroscopy,7, (2019) 39-56.
41. Rania Badry, Sherif El-Khodary, **Hanan Elhaes**, Nadra Nada and Medhat Ibrahim, “On the Molecular Modeling Analyses of Sodium Carboxymethyl Cellulose Treated with Acetic Acid”, Letters in Applied NanoBioScience, 8 (2), 2019, 553-557.
42. Ahmed M. Bayoumy, Gehan Youssif, Elzahraa A. Elgohary, Shimaa Husien, Heba Salah El Deen, Nourhan M. Albeltagy, Doaa R. Abdelnaby, Asmaa Medhat, **Hanan Elhaes** and Medhat A. Ibrahim “Impact of solvation on the geometrical parameters of some amino acids”, Letters in Applied NanoBioScience, 8 (2), 2019, 567-570.
43. Asmaa Ibrahim, **Hanan Elhaes**, Medhat Ibrahim, Ibrahim S. Yahia and Heba Y. Zahran,” Molecular Modeling Analyses for Polyvinylidene X (X=F, Cl, Br and I)”, Biointerface Research in Applied Chemistry, 9 (2) 2019, 3890-3893.
44. Paola Grenni, Anna Barra Caracciolo, Livia Mariani, Martina Cardoni, Cristina Riccucci, **Hanan Elhaes**, Medhat A. Ibrahim,”Effectiveness of a new green technology for metal removal from contaminated water”, Microchemical Journal, 147 (2019) 1010-1020
45. H. Abdelsalam, N.H. Teleb, I.S. Yahia, H.Y. Zahran, **H. Elhaes** and M.A. Ibrahim, “First principles study of the adsorption of hydrated heavy metals on graphene quantum dots”, J Phys Chem Solids, 130,(2) (2019), 32-40.
46. Hazem Abdelsalam, Vasil A. Saroka, Mohamed Ali, Nahed H. Teleb, **Hanan Elhaes**, Medhat A. Ibrahim,” Stability and electronic properties of edge functionalized silicene quantum dots: A first principles study”, Physica E: Low-dimensional Systems and Nanostructures, 108 (2019) 339–346.
- 2018**
47. Rania Badry, Alia S. A-E. Ghanem, Hend Ahmed, Ahmed Fahmy, **Hanan Elhaes**, Ahmed Refaat and Medhat Ibrahim,” Effect of Li, Na, K, Be, Mg and Ca on the electronic properties, geometrical parameters of carboxylic acids”, Biointerface Research in Applied Chemistry, 8(2018), 3657-3660.
48. Rania Badry, Amina Omar, Haitham Mohammed, Doha Adel Awies Mohamed, **Hanan Elhaes**, Ahmed Refaat, and Medhat Ibrahim,” Effect of Alkaline Elements on the Structure and Electronic properties of Glycine”, Biointerface Research in Applied Chemistry, 8 (2018), 3682-3687.
49. Rania Badry, Hassanein Shaban, **Hanan Elhaes**, Ahmed Refaat and Medhat Ibrahim, “Molecular Modeling Analyses of Polyaniline Substituted with Alkali and Alkaline Earth Elements”, Biointerface Research in Applied Chemistry, 8(2018), 3719-3724.
50. H. Ezzat, R. Badry, I.S. Yahia, H.Y. Zahran, **H. Elhaes** and M.A. Ibrahim, “Mapping the molecular electrostatic potential of carbon nanotubes”, Biointerface Research in Applied Chemistry. 8 (2018), 3539-3542.



Physics Department

51. M. A. Ibrahim, **H. Elhaes**, S. A. El-Khodary, M. Morsy, A. Refaat, I. S. Yahia and H. Y. Zahran, Molecular Modeling Analyses for the Effect of Alkali Metal Oxides on Graphene, Biointerface Research in Applied Chemistry. 8(2018), 3522-3525
52. **H. Elhaes**, H. Ezzat, M. Morsy, S. A. El-Khodary, I.S. Yahia, H.Y. Zahran, S. AlFaify and M.A. Ibrahim, "PVC/ZnO Nano Composite as Gas Sensor for Natural Gas", Sensor Lett. 16, 513–516 (2018)
53. **H. Elhaes**, N. A. Saleh, and M. A. Ibrahim "Molecular Modeling Applications of Some Bio-Polymers Blends as Biosensor", Sensor Lett. 16, 539–547 (2018)
54. **H. Elhaes**, H. Ezzat, R. Badry , I. S. Yahia, H. Y. Zahran, and M. A. Ibrahim, "The Interaction between Carbon Nanotube Decorated with CuO and ZnO and Hydrogen", Sensor Lett. 16, 445–453 (2018)
55. M. A. Hegazy, **H. Elhaes**, S. A. El-Khodary, M. Morsy, I. S. Yahia, H. Y. Zahran, S. AlFaify , and M. A. Ibrahim, " Molecular Modeling Analyses for ZnO/Graphene as Sensor for H<sub>2</sub>S ," Sensor Lett. 16, 71–75 (2018)
56. H. Ezzat, I.S. Yahia, H.Y. Zahran, S. AlFaify, R. Badry, **H. Elhaes** and M.A. Ibrahim, " Properties of Fullerene for the Detection of Halides: A Theoretical Approach ", Sensor Letters.16, (2018)217–223
57. Hazem Abdelsalam, **Hanan Elhaes**, Medhat A. Ibrahim, "First principles study of edge carboxylated graphene quantum dots", Physica B, 537, (2018) 77-86
58. Hazem Abdelsalam, **Hanan Elhaes**, Medhat A. Ibrahim, "Tuning electronic properties in graphene quantum dots by chemical functionalization: Density functional theory calculations", Chemical Physics Letters, (2018), 138-148.
59. Nabila S. Ammar, Walid El hotaby, Hanan S. Ibrahim, Sherif A. El-Khodary, **Hanan Elhaes** and Medhat A. Ibrahim, " Cost effective natural microspheres for the removal of Pb from wastewater", Current Metabolomics. 6 (2018) 40-45.
60. Abdel Aziz Mahmoud, Osama Osman ,**Hanan Elhaes**, Marco Ferretti, Ahmed Fakhry and Medhat A. Ibrahim "Computational Analyses for the Interaction Between Aspartic Acid and Iron", J. Comput. Theor. Nanosci. 15, 470–473 (2018)
61. FagrKh. Abdel-Gawad, Osama Osman, Samah M. Bassem, Hossam F. Nassar, Tarek A. Temraz, **Hanan Elhaes** and Medhat Ibrahim, (2018) "Spectroscopic Analyses and Genotoxicity of Dioxins in the Aquatic Environment of Alexandria", Marine Pollution Bulletin.127 (2), 618-625
- 2017**
- Book Chapters**
- Noha A. Saleh, **Hanan Elhaes**, Medhat Ibrahim, Viral Proteases and Their Inhibitors, Chapter 2: Design and Development of Some Viral Protease Inhibitors by QSAR and Molecular Modeling Studies, 2017, Pages 25-58
62. Hanan Elhaes, Ahmed Fakhry and **Medhat Ibrahim**, "Modeling the Interaction between Metal oxide/Carbon Nanotube and Ethanol", Sensor Lett.15(11), 604-607(2017)
63. Medhat Ibrahim, Kholmurzo T. Kholmurodov, Irina N. Fadeikina, Svetlana V. Morzhuhina, Evgeniya S. Popova, Hanan Elhaes and Abdel Aziz Mahmoud, "On the Molecular Modelling Structure of the Egyptian Soil/Sediment in River Nile Delta Region", J. Comput. Theor. Nanosci. 14 (8), 4133–4136 (2017).
64. Ahmed Fakhry, **Hanan Elhaes** and Medhat Ibrahim " Computational Notes on the Effect of Substitution on Fullerene", J. Comput. Theor. Nanosci. 14 (8), 4118–4120 (2017).



Physics Department

65. Medhat Ibrahim, **Hanan Elhaes** and Diaa Atta, "Computational Notes on the Effect of Sodium Substitution on the Physical Properties of Fullerene" J. Comput. Theor. Nanosci. 14 (8), 4114–4117 (2017).
66. Naziha Suliman Alghunaim, Amina Omar, **Hanan Elhaes** and Medhat Ibrahim, "Effect of ZnO and TiO<sub>2</sub> On the Reactivity of Some Polymers", J. Comput. Theor. Nanosci. 14 (8), 2838–2843 (2017)
67. Rasha A. Youness, Mohammed A. Taha, **Hanan Elhaes**, and Medhat Ibrahim "Preparation, FTIR Characterization and Mechanical Properties of Hydroxyapatite Nanopowders", J. Comput. Theor. Nanosci. 14 (5), (2017) 2409–2415.
68. Diaa Atta, Fathia Gomaa, **Hanan Elhaes** and Medhat Ibrahim, "Effect of Hydrated Dioxin on the Physical and Geometrical Parameters of Some Amino Acids", J. Comput. Theor. Nanosci. 14 (5), (2017) 2405–2408.
69. M. Hamdy El-Awady, Fathia Gomaa, **Hanan Elhaes** and Medhat Ibrahim, "Role of Carboxyl group in the coordination of metals in organic structures", J. Comput. Theor. Nanosci. 14 (5), (2017) 2341–2344.
70. Noha Saleh, Amany A. Mostafa, Amina Omar, **Hanan Elhaes** and Medhat Ibrahim, "Molecular Modeling Analyses of Modified Polyvinylalcohol/ Hydroxyapatite Composite", J. Comput. Theor. Nanosci. 14 (5), (2017) 2298–2301
71. Ali Okasha, Diaa Atta, Wael M. Badawy, Marina V. Frontasyeva, **Hanan Elhaes** and Medhat Ibrahim, "Modeling the Coordination between Na, Mg, Ca, Fe, Ni, and Zn with Organic Acids", J. Comput. Theor. Nanosci. 14 (3), 1357–1361 (2017).
72. Rasha A. Youness, Mohammed A. Taha, **Hanan Elhaes** and Medhat Ibrahim, "Molecular Modeling, FTIR Spectral Characterization and Mechanical Properties of Carbonated-Hydroxyapatite Prepared by Mechanochemical Synthesis" Materials Chemistry and Physics. 190 (2017) 209-218
- 2016**
73. Fathia Gomaa, Abdel Aziz Mahmoud, Diaa Atta, Medhat Ibrahim and **Hanan Elhaes**, "Interaction between Organic Acids and Aluminium Hydroxide", Energy and Environment Focus, 5, 330-333, (2016).
74. Diaa Atta, Fathia Gomaa, **Hanan Elhaes** and Medhat Ibrahim, "On the Molecular Modelling Analyses for the Effect of Hydrated Dioxin upon Organic Acids", Energy and Environment Focus, 5, 295-298, (2016).
75. Abdel-Baset H. Makky, **Hanan Elhaes**, Mohamed M. El-Okr, Ahmed Fakhry and Medhat Ibrahim, "Electrostatic Potential Maps of Fullerene C<sub>60</sub> and Some of its Specific Derivatives: DFT Approach", Quantum Matter 5, 287-290 (2016).
76. **H. Elhaes**, A. M. Bakry, S. Hassaballa, N. M. Elkashef, A. Fakhry and M. Ibrahim, "Effect of radiation on the structure of Chitosan: Modeling approach", Quantum Matter 5, 243-246 (2016).
77. A. Nassar, **H. Elhaes** and N. M. Elkashef, "Influences of Cold Rolling and Heat-Treatment on the Microstructure, Microhardness and Thermal Properties Al-Sn-Cu Alloy" Quantum Matter 5, 203-206 (2016).
- 2015**
78. Wessam Omara, Rehab Amin, **Hanan Elhaes**, Medhat Ibrahim and Souad A. Elfeky, 2015 "Preparation and Characterization of Novel Polyaniline Nanosensor for Sensitive Detection of Formaldehyde" Recent Patents on Nanotechnology, 9 (3): 195-203.
79. Noha Saleh, **Hanan Elhaes**, Zeinab Abdel Aziz and Medhat Ibrahim, "On the Spectroscopic Analyses of Aspartic Acid", Der Pharma Chemica. 7 (10) 219-222.
80. Medhat Ibrahim<sup>1</sup>, Osama Osman<sup>1</sup>, Abdel aziz Mahmoud<sup>1</sup> and **Hanan Elhaes**, 2015, "Spectroscopic analyses of water hyacinth: FTIR and modeling approaches", Der Pharma



Chemica, 7(9):182-188

81. Hanan Elhaes, Noha Saleh, Abdel Aziz Mahmoud, Osama Osman, Amina Omar and Medhat Ibrahim, **2015** "On the Spectroscopic Analyses of Fulleropyrrolidine-1-carbodithioic acid 2; 3 and 4-substituted-benzyl esters", Quantum Matter, 4, 594-598.
  82. Abdel-Baset H Mekky, **Hanan G Elhaes**, Mohamed M. El-Okr, Abdulaziz S Al-Aboodi and Medhat A. Ibrahim, **2015** "Effect of Solvents on the Electronic Properties of Fullerene Based Systems: Molecular Modelling", J Appl Computat Math, 4, 1-4 (2015).
  83. NA Saleh, **H Elhaes**, O Osman, AA Mahmoud, M Ibrahim, **2015** "Spectroscopic Analyses of Modified Fulleropyrrolidine Derivatives" The Open Spectroscopy Journal 9, 1-6.
  84. **HananElhaes**, Mohamed Attallah, Mohamed El-Okr, Mahmud Ibrahim, Ahmed Fakhry and Medhat Ibrahim, **2015** "Modeling the effect of some transition metal oxide on phosphate glass" Quantum Matter 4 (2), 123-126.
  85. **HananElhaes**, Abdullah Al-Hossain, Osama Hendawy and Medhat Ibrahim, **2015** "Modeling the effect of Salinity on Soil Organic Matter" Quantum Matter 4 (2), 94-97.
  86. Z Al-Fifi, NA Saleh, **HElhaes**, M Ibrahim, **2015** "On the Molecular Modeling Analyses of Novel HIV-1 Protease Inhibitors Based on Modified Chitosan Dimer" International Journal of Spectroscopy Volume 2015, Article ID 174098, 9 pages
  87. Aly Okascha, FathiaGomaa, **HananElhaes**, Mohamed Morsy, Sherif El-Khodary, Ahmed Fakhry and Medhat Ibrahim **2015** " Spectroscopic Analyses of the Photocatalytic Behavior of Nano Titanium Dioxide" SpectrochimicaActa Part A 136(2), 504-509.
- 2014**
88. **H. Elhaes**, S. El-khodary, M. Morsy, A. A. Fakhry and M. Ibrahim, **2014** "Application of TiO<sub>3</sub> as Gas Sensor: Modeling Approach", Sensor Letters, 12(8): 1325-1330.
  89. Abdel Aziz Mahmoud, Osama Osman, Walid El-hotaby, Ahmed Fakhry, Zainab Abdel Aziz, Medhat Ibrahim and **HananElhaes**, 2014 "Modeling and Molecular Spectroscopic Analyses of Cellulose " J. Appl. Sol. Chem. Model. 3 (3) 159-163.
  90. Abo-el-nourAbd-alla, Abdelmonam M. Hamdan, **HananElhaes** and Medhat Ibrahim, 2014 "Mathematical analysis of the reflection phenomenon of longitudinal waves at nano anisotropic thermo-piezoelectric medium", J. Comput. Theor. Nanosci. 11, 2329-2338.
  91. **HananElhaes**, Mohamed Attallah, YahiaElbashar, Ayser Al-Alousi, Mohamed El-Okr, Medhat Ibrahim, 2014 "Modeling and Optical Properties of P<sub>2</sub>O<sub>5</sub>-ZnO-CaO-Na<sub>2</sub>O Glasses Doped with Copper Oxide", J. Comput. Theor. Nanosci. 11(10), 2079-2084
  92. **HananElhaes**, MonazahKhafagi, Medhat Ibrahim, and Alaa El-Din A. Gawad, 2014 "Spectroscopic analyses of PVDX (X = F, Cl and Br)", J. Comput. Theor. Nanosci. 11(10), 2115-2119.
  93. **HananElhaes**, Noha Saleh, Amina Omar and Medhat Ibrahim, 2014 "Molecular Spectroscopic Study of FulleropyrrolidineCarbodithioic Acid", J. Comput. Theor. Nanosci. 11(10), 2136-2140.
  94. **H. Elhaes**, M. Attallah, Y. Elbashar, M. Ibrahim and M. El-Okr, 2014 "Application of Cu<sub>2</sub>O-doped phosphate glasses for bandpass filter", Physica B, 449, 251–254.
  95. **HananElhaes**, Abdel Aziz Mahmoud , Emad M. Ahmed, Mohamed S. Abdel-Aal, Osama Osman and Medhat Ibrahim, 2014" Development of Natural Blends for Removal of Organic Pollutants", J. Comput. Theor. Nanosci, 11(9), 1891- 1898.
  96. **HananElhaes**, FagrKh. Abdel-Gawad, Nahla M. Elkashef and Medhat Ibrahim, 2014 "Effect of Divalent Metals on the Molecular Structure of Protein: Modeling and Spectroscopic Approaches", J. Comput. Theor. Nanosci. 11, 1081-1085 (2014)



97. Abo-el-nour N. Abd-alla, Abdullah Y. Al-Hossain, **HananElhaes** and Medhat Ibrahim, 2014 "Reflection and Refraction of Waves in Nano-Smart Materials: Anisotropic Thermo-piezoelectric Materials", J. Comput. Theor. Nanosci. 11(3), 715-726.
98. Nabila S. Ammar, **HananElhaes**, Hanan S. Ibrahim, WalidMosaad and Medhat A. Ibrahim, 2014 " A Novel Structure for Removal of Pollutants from Wastewater" SpectrochimicaActa Part A. 121C, 216- 223.
- 2013**
99. **HananElhaes** and Medhat Ibrahim, 2013 "Exploring Materials: Molecular Modeling Approach" Rev. Theor. Sci. 1, 368-376.
100. **HananElhaes**, and Medhat Ibrahim, 2013 "Fullerene as Sensor for Halides: Modeling Approach "J. Comput. Theor. Nanosci. , 10, 2026- 2028.
101. Abdel-Baset H. Mekky, **HananElhaes**, Mohamed M. El-Oker and Medhat A. Ibrahim, 2013 "Electronic Properties of Substituted C59X (X= B, Al, Ga, In) Fullerene", Material Science An Indian Journal. 9(2) 50-55.
- 2012**
102. Abdel Aziz Mahmoud, **HananElHaes**, Osama Osman and Ihab M. Elkashef, 2012 "Molecular Spectroscopic investigation of Ismaillia Canal Sediment (Egypt) ", Journal of Applied Sciences Research, 8, 4045- 4050.
103. **HananElhaes**, AfafBabaier and Mohamed Abd El-Aal, 2012 " Studying the Polymerization of Aniline on Fullerene "The Open Spectroscopy Journal, 6, (Suppl 1: M2) 2-8.
104. Mohamed M. El-Okr, Abd el baset H. Makky, **HananElhaes** and Medhat A. Ibrahim, 2012 "Electronic Properties of Group V Substituted Fullerene: DFT Approach", International Journal of Scientific & Engineering Research 3 (8) 1-4.
105. **HananElhaes**, HananMoawad, and Medhat Ibrahim, 2012" Spectroscopic Analyses of the Chromium Interaction with Protein" J. Comput. Theor. Nanosci. , 9(8), 1036-1039.
106. **HananElhaes**, Osama Osman and Medhat Ibrahim, 2012 "Interaction of Nano Structure Material with Heme Molecule: Modelling Approach" J. Comput. Theor. Nanosci. ,9, 901–905.
107. Zarrag Al-Fifi, Entsar H. El-Araby and **HananElhaes** 2012" Monitoring of Radon Concentrations in Jazan Beach Soil", J. Appl. Sci. Res., 8(2): 823-827.
- 2011**
108. Abo-el-nour N. Abd-alla, Hassan a. Eshaq and **HananElhaes**, 2011" The phenomena of reflection and transmission waves in smart nano materials", J. Comput. Theor. Nanosci. , 8, 1670–1678.
109. **HananElhaes** and AfafBabaier, 2011 "Studying the Electronic Properties of Fullerene Alkali Dimers", J. Comput. Theor. Nanosci. , 8, 1509-1512.
110. **HananElhaes**, Mohamed Abd-El-Aal, Ahmed Refaat and Medhat Ibrahim, 2011 "Metal Interaction with Organic Acids: Semiempirical Molecular Modeling Approach", Australian Journal of Basic and Applied Sciences, 5(6): 44-50.
- 2010**
111. **HananElhaes**, AfafBabaeer and Medhat Ibrahim, 2010 "Effect of Metal Substitution on the Electronic Properties of Fullerene and Fullero-pyrrolidine" J. Comput. Theor. Nanosci. 7, 536-541.
- 2009**
112. Zarrag Al-Fifi, **HananElhaes**, and Medhat Ibrahim, 2009 "Cellulose Fiber/Nano Metal Oxide Composite: Spectroscopic and Modeling Analyses", Journal of Applied Sciences Research, 5(12), 2511-2514.
113. **HananElhaes**, Medhat Ibrahim, Mahmoud Sleim, Jinhui Liu, and Jiarui Huang, 2009 "SnO<sub>2</sub> as a Gas Sensor: Modeling and Spectroscopic Approach" SENSOR LETTERS, Vol. 7, 530–534.



Physics Department

- 114.** H. Elhaes 2009 "Studying the Physical Properties of Graphite and Diamond Using Molecular Modeling", J. Appl. Sci. Res., 5(1081-1077).
- 115.** M. Ibrahim, H. ElHaes, A. A. Khalil, A. F. Jalbout and A. de Leon, **2009** "Computational Notes on the Analysis of C59-Zn, C59-Cd, and C59-Hg Fullerenes", J. Comput. Theor. Nanosci. 6, 80–84.
- 116.** M. Ibrahim, H. ElHaes, A. J. Hameed, A. F. Jalbout and A. de Leon, **2009** "Analysis of C60 Doping with Gallium, Indium and Phosphorus Using Semiempirical Molecular Modelling ", J. Comput. Theor. Nanosci. 6, 85–88.
- 2008**
- 117.** M. Ibrahim, H. El-Haes, A. J. Hameed and A. F. Jalbout, **2008** "Structural and Electronic Properties of C60X6 (X= F, Cl, Br and I). A Theoretical Study", J. Comput. Theor. Nanosci. 5 (11), 2247-2251.
- 118.** M. Ibrahim, H. ElHaes, A. J. Hameed and A. H. Essa, **2008** " Spectroscopic Analysis of C80 Doping with Group III and Group V Elements Using Semiempirical PM3 Molecular Modelling Technique", Ecl. Quim, Sao Paulo, 30(1), 21-27.
- 2007**
- 119.** C. Hess, H. ElHaes, A. Waske, B. Buechner, C. Sekar, G. Krabbes, F. Heidrich-Meisner, and W. Brenig, **2007** "Linear Temperature Dependence of the Magnetic Heat Conductivity in CaCu2O3", Phys. Rev. Lett., 98, 027201-027204.
- 120.** Ali Jameel Hameed, Medhat Ibrahim and Hanan ElHaes, **2007** "Computational notes on structural and electronic properties of Fulleropyrrolidine-1-carbodithioic acid 2; 3 and 4-substituted-benzyl esters", J. Mol. Struct- THEOCHEM. 809 (2007) 131-136.
- 2006**
- 121.** M. Ibrahim and H. El-Haes, **2006** "Molecular Modeling Study of Nitromethane in Gas Phase", Bull. NRC, Egypt, 31(4) 269-277.
- 122.** M. Ibrahim, H. El-Haes, A. F. Jalbout, **2006**, "Semiempirical Molecular Modelling Study of C60 Doped with Silicon, Germanium and Aluminium", CJP. 44(6), 432-439.
- 123.** M. Ibrahim, M. Alaam, H. El-Haes A. F. Jalbout and A. de Leon, 2006, "Analysis of the Structure and Vibrational Spectra of Glucose and Fructose", Ecl. Quim., Sao Paulo, 31(3): 15-21.
- 124.** C. Hess, P. Ribeiro, B. Buechner, H. ElHaes, G. Roth, U. Ammerahl, and A. Revcolevschi, 2006, Magnon heat conductivity and mean free paths in two-leg spin ladders: A model-independent determination, Phys. Rev. B 73, 104407.
- 2005**
- 125.** M. Ibrahim and H. El-Haes, 2005 "Computational Spectroscopic Study of Copper, Cadmium, Lead and Zinc Interactions in the Environment", Int. J. Environment and Pollution, 23(4), 417-424.
- 126.** M. Ibrahim and H. El-Haes, 2005 "Spectroscopic Study of C60 and C80 and their Epoxides", CJP. 43(5), 915-923.
- 2004**
- 127.** C. Hess, H. ElHaes, B. Buechner, U. Ammerahl, M. Hucker, and A. Revcolevschi, 2004, "Magnon-Hole Scattering and Charge Order in Sr14-xCaxCu24O41", Phys. Rev. Lett. 93, 027005.