

CURRICULUM VITAE

PERSONAL DATA

Name	Rageh Attia Khalifa Hussein
Nationality	Egyptian
Position	Instructor
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EDUCATION

Year	Academic Degree	Institution
2001	B.Sc. Degree in physics	Ain Shams University, Egypt
2005	Graduate school of theoretical physics	Ain Shams University, Egypt
2009	M.Sc. Degree in theoretical physics	Ain Shams University, Egypt
2016	Ph.D. degree in solid state physics	Zagazig University. Egypt.

WORK EXPERIENCE

Period	Position	Address
2010-till now	Instructor	Science College, Department of Physics, Imam Muhammad Ibn Saud Islamic University, Riyadh, KSA.

RESEARCH INTERESTS

Molecular Modling, Materials Science

PUBLICATIONS

- Theoretical investigations for electronic structures and photo dissociation of bromine molecule, International Journal of the Physical Sciences Vol. 5 (7), pp. 978-983, July 2010.
- First Principles' Investigation of Electronic Properties of Hf, Ag, Cd, Zn, Ce, Nd, Sm-Modified Lead Zirconate Titanate, Journal of Computational and Theoretical Nanoscience Vol. 13, 7661–7665, 2016.
- Theoretical Investigation of Susceptibility to Fatigue for Modified Lead Zirconate Titanate, Quantum Matter Vol. 5, 709-712, 2016.
 - Pseudo-Jahn-Teller Effect as an Approach to Investigate the Enhancement of Ferroelectricity for Gold-Modified PZT, Quantum Matter Vol. 5, 713-716, 2016.
- Molecular structure, frontier molecular orbital and spectral analysis of dimethylamino chalcones efficient lasing dyes, Journal of Molecular Structure Vol.1178, 285-289, 2019.
- Experimental and theoretical study of the structure, frontier molecular orbital, tautomerism and spectral analysis of 3-(p-substituted phenyl)-5-phenyl-1H-pyrazole. Journal of Molecular Liquids 287 (2019) 110675.
- DFT Investigation of Structural and Electronic Properties of Modified PZT. ACTA CHEMICA IASI, 27_1, 15-30 (2019).
- DFT Investigation of Geometric Structure, IR and Raman Spectra of Vinyl Halides CH₂=CH-X (X IS F, Cl AND Br) 37-Vol.-10-Issue-12-Dec-2019-IJPSR-5537-5544.
- Density Functional Theory Investigation of Some Pyridine Dicarboxylic Acids Derivatives as Corrosion Inhibitors, Int. J. Electrochem. Sci., 15 (2020) 4274 – 4286.
- Molecular Dynamics Investigation for the Impact of Metakaolin on mechanical Properties of the Ordinary Portland Cement. IJPSR, Volume 11, Issue 10, 2020 .
- Theoretical and Experimental Studies of Different Amine Compounds as Corrosion Inhibitors for Aluminum in Hydrochloric Acid. Biointerface Research in Applied Chemistry. Volume 11, Issue 2, 2021.
- Molecular docking identification for the efficacy of some zinc complexes with chloroquine and hydroxychloroquine against main protease of COVID-19. Journal of Molecular Structure, Volume 1231, 5 May 2021.
- Density Functional Theory and Molecular Docking Investigations of the Chemical and Antibacterial Activities for 1-(4-Hydroxyphenyl)-3-phenylprop-2-en-1-one. Molecules 2021, 26, 3631
- DFT, ADMET and Molecular Docking Investigations for the Antimicrobial Activity of 6,6'-Diamino-1,1',3,3'-tetramethyl-5,5'-(4-chlorobenzylidene)bis[pyrimidine-2,4(1H,3H)-dione]. Molecules 2022, 27, 620.
- Intermolecular CH-π Electrons Interaction in Poly (9, 9-dioctylfluorenyl-2, 7-diyl) (PFO): An Experimental and Theoretical Study. Molecules 2022, 27(5), 1488.
- Probing the Action of Screened Anticancer Triazole–Tetrazole Derivatives against COVID-19 Using Molecular Docking and DFT Investigations. Natural Product Communications Volume 17(5): 1–10.

