

## Assoc. Prof. MUSTAFA KURBAN

### Personal Information

**Office Phone:** [+90 312 381 2350](tel:+903123812350) Extension: 6598

**Fax Phone:** [+90 312 381 2355](tel:+903123812355)

**Email:** kurbanm@ankara.edu.tr

**Other Email:** mkurbanphys@gmail.com

**Web:** <https://avesis.ankara.edu.tr/kurbanm>

**Address:** Fatih Caddesi No:197/7 PK:06290 Keçiören/ANKARA

### International Researcher IDs

ScholarID: -xcZFYwAAAAJ

ORCID: 0000-0002-7263-0234

Publons / Web Of Science ResearcherID: P-8494-2019

ScopusID: 56940375000

Yoksis Researcher ID: 134821

### Biography

Mustafa Kurban is an Associate Professor in the Department of Prosthetics & Orthotics at [Ankara University](https://www.ankara.edu.tr). He earned his Ph.D. in Physics from [Middle East Technical University](https://www.metu.edu.tr) in 2016 and pursued a postdoctoral position in Materials Science & Engineering at the [University of California, Riverside](https://www.ucr.edu), from 2018 to 2019. His diverse research portfolio encompasses energy storage, sensors, bulk heterojunction solar cells, the application of machine learning in materials science, optics, drug delivery systems, nanomaterials, 2D materials, organic molecules, and crystal structures.

### Education Information

Post Doctorate, University of California, Riverside, Materials Science & Engineering, United States Of America 2018 - 2019

Doctorate, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Physics, Turkey 2010 - 2016

### Research Areas

Health Sciences, Natural Sciences, Engineering and Technology

### Academic Titles / Tasks

Associate Professor, Ankara University, Sağlık Bilimleri Fakültesi, Ortez-Protez Bölümü, 2023 - Continues

Associate Professor, Kirşehir Ahi Evran University, Faculty of Engineering and Architecture, Electrical - electronics Engineering, 2020 - 2023

Assistant Professor, Kirşehir Ahi Evran University, Vocational School of Technical Sciences, Department of Electronics and Automation, 2017 - 2020

Research Assistant, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Physics, 2010 - 2016

## Academic and Administrative Experience

Manager of Research and Application Center, Kirşehir Ahi Evran University, 2019 - 2023

## Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Drug delivery potential of carbon and boron nitride nanotubes: A DFT-D3 analysis of curcumin binding interactions**  
Bechohra L. L., KURBAN M., Medigue N. E. H., Kellou-Taïri S.  
Diamond and Related Materials, vol.149, 2024 (SCI-Expanded)
- II. **Elucidating roles of fulleropyrrolidine-based materials as extraordinary electron transporters for boosting efficiency of perovskite photovoltaics**  
Kurban M., Shariatinia Z.  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, vol.194, pp.112220, 2024 (SCI-Expanded)
- III. **Computational study of new small molecules D-A based on triphenylamines for bulk heterojunction solar cells (BHJ)**  
Mouhi R. E., Slimi A., Khattabi S. E., Benjelloun A. T., Fitri A., Benzakour M., Mcharfi M., KURBAN M.  
Computational and Theoretical Chemistry, vol.1241, 2024 (SCI-Expanded)
- IV. **Enhancing the electronic properties of TiO<sub>2</sub> nanoparticles through carbon doping: An integrated DFTB and computer vision approach**  
KURBAN M., Polat C., Serpedin E., Kurban H.  
Computational Materials Science, vol.244, 2024 (SCI-Expanded)
- V. **Rational and green functionalization of B,N-C<sub>60</sub> by DNA bases devised as incredible electron transport compounds for perovskite photovoltaic devices**  
Shariatinia Z., KURBAN M.  
Materials Today Communications, vol.39, 2024 (SCI-Expanded)
- VI. **Investigating the effect of Zn doping and temperature on the photoluminescence behaviour of CuLaSe<sub>2</sub> quantum dots**  
Çadırcı M., Elibol E., Demirci T., KURBAN M.  
Luminescence, vol.39, no.4, 2024 (SCI-Expanded)
- VII. **Rational design of SnO<sub>2</sub> thin film coated cathode with function of entrapping polysulfides for performance enhanced Li-S batteries**  
Shang R., KURBAN M., ma Y., Ozkan M., Ozkan C. S.  
Journal of Power Sources, vol.597, 2024 (SCI-Expanded)
- VIII. **Chelant-enhanced solution for wafer-scale synthesis of few-layer WS<sub>2</sub> films**  
Isarraraz M., Pena P., Sayyad M., Yang S., Li H., Akhavi A., Rashetnia M., Shang R., Coley W., Cui Y., et al.  
MRS BULLETIN, vol.48, no.10, pp.1073-1085, 2023 (SCI-Expanded)
- IX. **Size-dependent adsorption performance of ZnO nanoclusters for drug delivery applications**  
Kurban M., Muz I.  
STRUCTURAL CHEMISTRY, vol.34, no.3, pp.1061-1071, 2023 (SCI-Expanded)
- X. **Sulfur doping concentration effect on the electronic and structural properties of ZnO nanoparticles: Insights from DFTB calculations**  
Kurban M.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1224, 2023 (SCI-Expanded)
- XI. **Superporous nanocarbon materials upcycled from polyethylene terephthalate waste for scalable energy storage**  
Mirjalili A., Dong B., Zerrin T., Akhavi A., Kurban M., Ozkan C. S., Ozkan M.  
JOURNAL OF ENERGY STORAGE, vol.58, 2023 (SCI-Expanded)
- XII. **A strategy to enhance V-OC of pi-conjugated molecules based on thieno[2,3-b] indole for applications in bulk heterojunction organic solar cells using DFT, TD-DFT, and 3D-QSPR modeling**

## studies

El Mouhi R., Daoui O., Fitri A., Benjelloun A. T., El Khattabi S., Benzakour M., Mcharfi M., Kurban M.  
NEW JOURNAL OF CHEMISTRY, vol.47, no.2, pp.812-827, 2023 (SCI-Expanded)

- XIII. **Zinc oxide nanoclusters and their potential application as CH<sub>4</sub> and CO<sub>2</sub> gas sensors: Insight from DFT and TD-DFT**  
Muz I., Kurban M.  
JOURNAL OF COMPUTATIONAL CHEMISTRY, vol.43, no.27, pp.1839-1847, 2022 (SCI-Expanded)
- XIV. **Rapidly predicting Kohn-Sham total energy using data-centric AI**  
Kurban H., Kurban M., Dalkilic M. M.  
SCIENTIFIC REPORTS, vol.12, no.1, 2022 (SCI-Expanded)
- XV. **DFT, DFTB and TD-DFT theoretical investigations of p-conjugated molecules based on thieno[2,3-b] indole for dye-sensitized solar cell applications**  
El Mouhi R., Slimi A., Fitri A., Benjelloun A. T., ElKhattabi S., Benzakour M., Mcharfi M., Kurban M.  
PHYSICA B-CONDENSED MATTER, vol.636, 2022 (SCI-Expanded)
- XVI. **A density functional theory study on favipiravir drug interaction with BN-doped C<sub>60</sub> heterofullerene**  
Muz I., GÖKTAŞ F., Kurban M.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.135, 2022 (SCI-Expanded)
- XVII. **A first-principles evaluation on the interaction of 1,3,4-oxadiazole with pristine and B-, Al-, Ga-doped C-60 fullerenes**  
Muz I., Kurban M.  
JOURNAL OF MOLECULAR LIQUIDS, vol.335, 2021 (SCI-Expanded)
- XVIII. **Building Machine Learning systems for multi-atoms structures: CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite nanoparticles**  
Kurban H., Kurban M.  
COMPUTATIONAL MATERIALS SCIENCE, vol.195, 2021 (SCI-Expanded)
- XIX. **Sensing capability and diameter-dependent electronic structure of boron nitride nanotubes**  
Muz I., Alaei S., Kurban M.  
MATERIALS TODAY COMMUNICATIONS, vol.27, 2021 (SCI-Expanded)
- XX. **Rare-class learning over Mg-doped ZnO nanoparticles**  
Kurban H., Kurban M.  
CHEMICAL PHYSICS, vol.546, 2021 (SCI-Expanded)
- XXI. **Effect of Mg content on electronic structure, optical and structural properties of amorphous ZnO nanoparticles: A DFTB study**  
Kurban H., Alaei S., Kurban M.  
JOURNAL OF NON-CRYSTALLINE SOLIDS, vol.560, 2021 (SCI-Expanded)
- XXII. **A DFT study on stability and electronic structure of AlN nanotubes**  
Muz I., Kurban H., Kurban M.  
MATERIALS TODAY COMMUNICATIONS, vol.26, 2021 (SCI-Expanded)
- XXIII. **Single- and multi-layer arsenene as an anode material for Li, Na, and K-ion battery applications**  
Kanli M., Kurban M., Ozdemir B., Onen A., Durgun E.  
COMPUTATIONAL MATERIALS SCIENCE, vol.186, 2021 (SCI-Expanded)
- XXIV. **Electronic structures and bonding of graphdiyne and its BN analogs: Transition from quasi-planar to planar sheets**  
Muz I., Kurban M.  
JOURNAL OF ALLOYS AND COMPOUNDS, vol.846, 2020 (SCI-Expanded)
- XXV. **Size dependence in the electronic and optical properties of a BN analogue of two-dimensional graphdiyne: A theoretical study**  
Muz I., Goktaa F., Kurban M.  
CHEMICAL PHYSICS, vol.539, 2020 (SCI-Expanded)
- XXVI. **The electronic structure, transport and structural properties of nitrogen-decorated graphdiyne nanomaterials**

- Muz I, Kurban M.  
JOURNAL OF ALLOYS AND COMPOUNDS, vol.842, 2020 (SCI-Expanded)
- XXVII. **Tailoring the structural properties and electronic structure of anatase, brookite and rutile phase TiO<sub>2</sub> nanoparticles: DFTB calculations**  
Kurban H., Dalkilic M., TEMİZ S., Kurban M.  
COMPUTATIONAL MATERIALS SCIENCE, vol.183, 2020 (SCI-Expanded)
- XXVIII. **DFT and TD-DFT studies of new pentacene-based organic molecules as a donor material for bulk-heterojunction solar cells**  
Muz I, Kurban M., Dalkilic M.  
JOURNAL OF COMPUTATIONAL ELECTRONICS, vol.19, no.3, pp.895-904, 2020 (SCI-Expanded)
- XXIX. **Theoretical investigation of the adsorption behaviors of fluorouracil as an anticancer drug on pristine and B-, Al-, Ga-doped C<sub>36</sub> nanotube**  
Kurban M., Muz I.  
JOURNAL OF MOLECULAR LIQUIDS, vol.309, 2020 (SCI-Expanded)
- XXX. **Electronic Transport and Non-linear Optical Properties of Hexathiopentacene (HTP) Nanorings: A DFT Study**  
Muz I, Kurban M.  
JOURNAL OF ELECTRONIC MATERIALS, vol.49, no.5, pp.3282-3289, 2020 (SCI-Expanded)
- XXXI. **A combined experimental and DFT/TD-DFT studies on the electronic structure, structural and optical properties of quinoline derivatives**  
Kurban M., Sertbakan T. R., Gunduz B.  
JOURNAL OF MOLECULAR MODELING, vol.26, no.6, 2020 (SCI-Expanded)
- XXXII. **Evaluation of electronic transport and optical response of two-dimensional Fe-doped TiO<sub>2</sub> thin films for photodetector applications**  
Kara F., Kurban M., Coskun B.  
OPTIK, vol.210, 2020 (SCI-Expanded)
- XXXIII. **Suppression of the Shuttle Effect in Li-S Batteries via Magnetron Sputtered TiO<sub>2</sub> Thin Film at the Electrode-Electrolyte Interface**  
Zerrin T., Kurban M., Dickson M. M., Ozkan M., Ozkan C. S.  
ACS APPLIED ENERGY MATERIALS, vol.3, no.2, pp.1515-1529, 2020 (SCI-Expanded)
- XXXIV. **3d-transition metals (Cu, Fe, Mn, Ni, V and Zn)-doped pentacene pi-conjugated organic molecule for photovoltaic applications: DFT and TD-DFT calculations**  
Muz I, GÖKTAŞ F., Kurban M.  
THEORETICAL CHEMISTRY ACCOUNTS, vol.139, no.2, 2020 (SCI-Expanded)
- XXXV. **Molecular dynamics study on composition and temperature dependences of mechanical properties of CdTeSe nanowires under uniaxial stretching**  
Koyluoglu B., Alaei S., Kurban M.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.33, no.31, 2019 (SCI-Expanded)
- XXXVI. **Density-functional tight-binding approach for the structural analysis and electronic structure of copper hydride metallic nanoparticles**  
Kurban H., Kurban M., Dalkilic M.  
MATERIALS TODAY COMMUNICATIONS, vol.21, 2019 (SCI-Expanded)
- XXXVII. **A comprehensive study on electronic structure and optical properties of carbon nanotubes with doped B, Al, Ga, Si, Ge, N, P and As and different diameters**  
Muz I, Kurban M.  
JOURNAL OF ALLOYS AND COMPOUNDS, vol.802, pp.25-35, 2019 (SCI-Expanded)
- XXXVIII. **A study of structural phase transitions and optoelectronic properties of perovskite-type hydride MgFeH<sub>3</sub>: ab initio calculations**  
Kurban M., Kurkcu C., Yamcicler C., GÖKTAŞ F.  
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.31, no.30, 2019 (SCI-Expanded)
- XXXIX. **Enhancement of electronic, photophysical and optical properties of 5,5'-Dibromo-2,2'-bithiophene**

**molecule: new aspect to molecular design**

Muz I, Kurban M.

OPTO-ELECTRONICS REVIEW, vol.27, no.2, pp.113-118, 2019 (SCI-Expanded)

- XL. **Tunable electronic structure and structural transition of GaAs clusters at high pressure and temperature**  
Kurban M.  
JOURNAL OF ALLOYS AND COMPOUNDS, vol.791, pp.1159-1166, 2019 (SCI-Expanded)
- XLI. **Structural evolution and electronic properties of CaS: An ab initio study**  
Kurkcu C., Yamcicler C., Kurban M.  
SOLID STATE SCIENCES, vol.90, pp.14-20, 2019 (SCI-Expanded)
- XLII. **Experimental and theoretical studies of the structural, electronic and optical properties of BCzVB organic material**  
Kurban M., Gunduz B., GÖKTAŞ F.  
OPTIK, vol.182, pp.611-617, 2019 (SCI-Expanded)
- XLIII. **Photophysical, spectroscopic properties and electronic structure of BND: Experiment and theory**  
Sas E. B., Kurban M., Gunduz B., Kurt M.  
SYNTHETIC METALS, vol.246, pp.39-44, 2018 (SCI-Expanded)
- XLIV. **Photophysical and optical properties of 5-Bromo-2-nitropyridine organic molecule: Experiment and theory**  
Gunduz B., Kurban M.  
OPTICAL MATERIALS, vol.85, pp.373-381, 2018 (SCI-Expanded)
- XLV. **Electronic structure, elastic and phonon properties of perovskite-type hydrides MgXH<sub>3</sub> (X = Fe, Co) for hydrogen storage**  
Candan A., Kurban M.  
SOLID STATE COMMUNICATIONS, vol.281, pp.38-43, 2018 (SCI-Expanded)
- XLVI. **Investigation of Structural, Vibrational Properties and Electronic Structure of Fluorene-9-Bisphenol: A DFT Approach**  
Kotiloglu S. O., Celik S., Tanis E., Kurban M.  
CHEMISTRYSELECT, vol.3, no.21, pp.5934-5940, 2018 (SCI-Expanded)
- XLVII. **Photonic, spectroscopic properties and electronic structure of PTCDI-C8 organic nanostructure**  
Gunduz B., Kurban M.  
VIBRATIONAL SPECTROSCOPY, vol.96, pp.46-51, 2018 (SCI-Expanded)
- XLVIII. **Ab initio study of structural and electronic properties of SinC5-nH8 (n=0-5) series: Probing the 2D to 3D structural transition**  
Muz I, Kurban M.  
INORGANICA CHIMICA ACTA, vol.477, pp.318-325, 2018 (SCI-Expanded)
- XLIX. **Analysis of the geometrical properties and electronic structure of arsenide doped boron clusters: Ab-initio approach**  
Muz I, Kurban M., Sanli K.  
INORGANICA CHIMICA ACTA, vol.474, pp.66-72, 2018 (SCI-Expanded)
- L. **The structural, electronic and spectroscopic properties of 4FPBAPE molecule: Experimental and theoretical study**  
Tanis E., Sas E. B., Kurban M., Kurt M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1154, pp.301-318, 2018 (SCI-Expanded)
- LI. **Electronic structure, optical and structural properties of Si, Ni, B and N-doped a carbon nanotube: DFT study**  
Kurban M.  
OPTIK, vol.172, pp.295-301, 2018 (SCI-Expanded)
- LII. **Study of structural, optical properties and electronic structure of PTCDI-C5 organic nanostructure**  
Kurban M., Gunduz B.  
CHEMICAL PHYSICS LETTERS, vol.691, pp.14-21, 2018 (SCI-Expanded)

- LIII. **Electronic structure, optical and structural properties of organic 5,5'-Dibromo-2,2'-bithiophene**  
Kurban M., Gunduz B.  
OPTIK, vol.165, pp.370-379, 2018 (SCI-Expanded)
- LIV. **Physical and optical properties of DCJTB dye for OLED display applications: Experimental and theoretical investigation**  
Kurban M., Gunduz B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1137, pp.403-411, 2017 (SCI-Expanded)
- LV. **Segregation formation, thermal and electronic properties of ternary cubic CdZnTe clusters: MD simulations and DFT calculations**  
Kurban M., Erkoç S.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.88, pp.243-251, 2017 (SCI-Expanded)
- LVI. **Mechanical properties of CdZnTe nanowires under uniaxial stretching and compression: A molecular dynamics simulation study**  
Kurban M., Erkoç S.  
COMPUTATIONAL MATERIALS SCIENCE, vol.122, pp.295-300, 2016 (SCI-Expanded)
- LVII. **Microstructural properties and local atomic structures of cobalt oxide nanoparticles synthesised by mechanical ball-milling process**  
Akgül F. A., Akgül G., Kurban M.  
PHILOSOPHICAL MAGAZINE, vol.96, no.30, pp.3211-3226, 2016 (SCI-Expanded)
- LVIII. **Structural and thermal properties of Cd-Zn-Te ternary nanoparticles: Molecular-dynamics simulations**  
Kurban M., MALCIOĞLU O. B., Erkoç S.  
CHEMICAL PHYSICS, vol.464, pp.40-45, 2016 (SCI-Expanded)
- LIX. **Structural and Electronic Properties of  $Zn_mCd_nTe_k$  ( $m+n+k=2-4$ ) Clusters: DFT Calculations**  
Kurban M., Erkoç S.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.12, no.9, pp.2605-2615, 2015 (SCI-Expanded)
- LX. **Quantum dynamics of  $H(S-2) + FO((2)Pi) \rightarrow HF((1)Sigma(+)) + O(P-3)$  reaction on the  $1(3)A'$  state**  
Kurban M., GÖKTAŞ F., Karabulut E., Tutuk R.  
MOLECULAR PHYSICS, vol.109, no.5, pp.789-795, 2011 (SCI-Expanded)
- LXI. **Time-Dependent Quantum Study of  $H(S-2)+FO((2)Pi) \rightarrow OH((2)Pi)+F(P-2)$  Reaction on the  $1(3)A'$  and  $1(3)A''$  States**  
GÖKTAŞ F., Tutuk R., Kurban M.  
JOURNAL OF COMPUTATIONAL CHEMISTRY, vol.31, no.14, pp.2607-2611, 2010 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Controlling structural and electronic properties of ZnO NPs: Density-functional tight-binding method**  
KURBAN M., KURBAN H., Dalkılıç M.  
Bilge International Journal of Science and Technology Research, vol.3, pp.35-39, 2019 (Peer-Reviewed Journal)
- II. **The effects of a single atom substitution and temperature on electronic and photophysical properties F8T2 organic material**  
KURBAN M.  
Bilge International Journal of Science and Technology Research, vol.3, pp.40-44, 2019 (Peer-Reviewed Journal)
- III. **Study of Structural and Optoelectronic Properties of Hexagonal ZnO Nanoparticles**  
KURBAN H., Kurban M.  
Bilecik Şeyh Edebali Üniversitesi Fen Bilimleri Dergisi, vol.6, no.2, pp.243-250, 2019 (Peer-Reviewed Journal)
- IV. **MOLECULAR DYNAMICS STUDY ON THE STRUCTURAL, THERMAL AND ENERGETIC PROPERTIES OF**

## **GaAs NANOPARTICLES**

KURBAN M.

Eskişehir Technical University Journal of Science and and Technology A- Applied Sciences and Engineering, vol.19, no.3, pp.620-627, 2018 (Peer-Reviewed Journal)

V. **Size- and composition-dependent structure of ternary Cd-Te-Se nanoparticles**

Kurban M.

TURKISH JOURNAL OF PHYSICS, vol.42, no.4, pp.443-454, 2018 (ESCI)

VI. **Investigation of the Structural Properties of CdTe and ZnTe Binary Nanorods Under Heat Treatment Molecular Dynamics Simulations**

KURBAN M., ŞAKŞİR E.

Quantum Matter, vol.5, no.4, pp.602-606, 2016 (Peer-Reviewed Journal)

VII. **Structural properties of  $Zn_xCd_{1-x}Te$  0.25/0.50 and 0.75 ternary nanorods Molecular Dynamics Simulations**

KURBAN M., ERKOÇ Ş.

Research and Reviews: Journal of Pure and Applied Physics, vol.1, no.4, pp.35-42, 2013 (Peer-Reviewed Journal)

## **Books & Book Chapters**

I. **Ternary II-VI Alloys Promising for Application in Photodetectors**

KURBAN M., MALCIOĞLU O. B., Erkoç Ş.

in: Handbook of II-VI Semiconductor-Based Sensors and Radiation Detectors, Ghenadii Korotcenkov, Editor, Springer, Cham, Cham, pp.87-106, 2023

II. **II-VI Semiconductors Bandgap Engineering**

KURBAN M., ŞİMŞEK Y., Erkoç Ş.

in: Handbook of II-VI Semiconductor-Based Sensors and Radiation Detectors, Ghenadii Korotcenkov, Editor, Springer, Cham, Cham, pp.109-131, 2023

## **Refereed Congress / Symposium Publications in Proceedings**

I. **Potential of Carbon and Boron Nitride Nanotubes for Drug Delivery Established by Analysis of Curcumin-Nanotubes Binding Interactions : A DFT Investigation**

BECHOHRA L. L., KURBAN M., MEDIGUE N. E. H., KELLOU-TAIRI S.

2nd National Conference on Materials Sciences and Engineering (MSE'23), Maghnia, Algeria, 12 December 2023

II. **Effect of Sulfur Doping on Electronic Structure of ZnO Nanoparticles**

MUZ İ., KURBAN M.

5th International Eurasian Conference on Biological and Chemical Sciences, Ankara, Turkey, 23 November 2022

III. **Predicting Atom Types of Anatase TiO<sub>2</sub> Nanoparticles with Machine Learning**

KURBAN H., KURBAN M., Sharma P., Dalkılıç M.

International Conference on Engineering and Innovative Materials, Singapore, 4 - 06 September 2020, vol.880, pp.89-94

IV. **Functionalized graphdiyne: Size-Dependent electronic and optical properties based on DFTB**

KURBAN M., MUZ İ.

3rd International Conference on Physical Chemistry and Functional Materials, Malatya, Turkey, 22 - 24 September 2020

V. **Structural and electronic properties of favipiravir drug adsorption on the C<sub>30</sub>B<sub>15</sub>N<sub>15</sub> heterofullerene: DFT studies**

MUZ İ., KURBAN M.

3rd International Conference on Physical Chemistry and Functional Materials, Malatya, Turkey, 22 - 24 September 2020

- VI. **INVESTIGATION OF ELECTRONIC STRUCTURE AND THERMAL PROPERTIES OF NANO-SATURN FOR FUNCTIONAL MATERIALS**  
KURBAN M.  
ADIM PHYSICS DAYS VIII, 12 - 15 August 2019, pp.142-151
- VII. **Investigation of Electrical and Structural Properties of ZrO<sub>2</sub> Thin Films**  
COŞKUN B., KURBAN M.  
6th International Conference on Materials Science and Nanotechnology for Next Generation (MSNG2019), Niğde, Turkey, 16 - 18 December 2019, pp.349-351
- VIII. **Size Dependent Electronic Structure and Structural Properties of Cupric Oxide (CuO) Nanoparticles**  
KURBAN H., KURBAN M., Dalkılıç M.  
International Natural Science, Engineering and Material Technologies Conference, İstanbul, Turkey, 9 - 10 September 2019
- IX. **The Effects of a Single Atom Substitution and Temperature on Electronic and Photophysical Properties F8T2 Organic Material**  
KURBAN M.  
2nd International Conferences on Science and Technology Natural Science and Technology, 26 - 30 August 2019, pp.31-38
- X. **Controlling Structural and Electronic Properties of ZnO NPs: Density-Functional Tight-Binding Method**  
KURBAN M., KURBAN H., Dalkılıç M.  
2nd International Conferences on Science and Technology Natural Science and Technology, Prizren, Serbia, 26 - 30 August 2019, pp.23-30
- XI. **Assessment of Long-Range Corrected (LC) Parameters for Prediction of Electronic Structure of Carbazole**  
KURBAN M.  
International Natural Science, Engineering and Material Technologies Conference, İstanbul, Turkey, 9 - 10 September 2019
- XII. **Band Engineering and Photophysical Properties of C-Doped F8T2 Organic Compound**  
KURBAN M., COŞKUN B.  
International Natural Science, Engineering and Material Technologies Conference, 9 - 10 September 2019
- XIII. **A DFT comparative study of electronic properties on pristine single walled carbon nanotubes**  
MUZ İ., KURBAN M.  
International Conference on Materials Science, Mechanical and Automotive Engineerings and Technology, Nevşehir, Turkey, 21 - 23 June 2019
- XIV. **Electronic properties of (4,4) carbon nanotube via 3A, 4A and 5A group atoms doping**  
MUZ İ., KURBAN M.  
2nd International Conference on Physical Chemistry and Functional Materials, Nevşehir, Turkey, 25 - 27 June 2019
- XV. **Predicting Chemical Bioavailability of Fluoxastrobin by DFT calculations**  
TANIŞ E., KURBAN M., ÖZKAN KOTİLOĞLU S., ÇELİK S.  
International Congress on the World of Technology and Advanced Materials (WITAM-2018), Kırşehir, Turkey, 21 - 23 September 2018, pp.16
- XVI. **Investigation of photophysical and toxicity properties of Pyraclostrobin**  
ÇELİK S., TANIŞ E., ÖZKAN KOTİLOĞLU S., KURBAN M.  
International Congress on the World of Technology and Advanced Materials (WITAM-2018), Kırşehir, Turkey, 21 - 23 September 2018, pp.33
- XVII. **Evaluation of Performance of Functionals to Estimate Charge Transport Properties and Excited-State Energies**  
BABUR ŞAŞ E., KURBAN M., GÜNDÜZ B., KURT M.  
International Congress on the World of Technology and Advanced Materials (WITAM-2018), Kırşehir, Turkey, 21 - 23 September 2018
- XVIII. **Structural, thermal and vibrational properties of poly-hexamethylene biguanide hydrochloride**



**(PHMB)**

ÇELİK S., KURBAN M., ÖZKAN KOTİLOĞLU S., TANIŞ E.

International Congress on the World of Technology and Advanced Materials (WITAM-2018), Kırşehir, Turkey, 21 - 23 September 2018

- XIX. **Electronic Structure, Optical and Spectroscopic Properties of BCzVB Organic Molecule**  
GÜNDÜZ B., KURBAN M.  
International Conference on Physical Chemistry and Functional Materials (PCFM'xx18), Elazığ, Turkey, 19 - 21 June 2018, pp.315
- XX. **Controlling Photophysical Properties and Electronic Structure of PTCDI-C8 Nanostructure**  
GÜNDÜZ B., KURBAN M.  
International Conference on Physical Chemistry and Functional Materials (PCFM'xx18), Elazığ, Turkey, 19 - 21 June 2018, pp.3-5
- XXI. **Effects of Doped Atoms on the Structural, Electronic and Optical Properties of a Carbon Nanotube**  
KURBAN M., GÖKTAŞ F.  
4TH INTERNATIONAL CONFERENCE ON ENGINEERING AND NATURAL SCIENCES, Kiev, Ukraine, 2 - 06 May 2018
- XXII. **Unusual structural phase transition properties of GaAs Clusters under pressure**  
KURBAN M., KÜRKÇÜ C.  
4TH INTERNATIONAL CONFERENCE ON ENGINEERING AND NATURAL SCIENCES, Kiev, Ukraine, 2 - 06 May 2018, pp.509
- XXIII. **2D-3D STRUCTURAL TRANSITION IN  $\text{Si}_n\text{C}_5\text{-nH}_8$  (n=0-5) SERIES**  
MUZ İ., KURBAN M.  
International Conference on Material Science and Technology in Cappadocia (IMSTEC'17), 11 - 13 October 2017
- XXIV. **UNDERSTANDING THE STRUCTURAL PROPERTIES OF CdTeSe NANOPARTICLES FOR SOLAR CELL APPLICATIONS**  
KURBAN M., MUZ İ.  
International Conference on Material Science and Technology in Cappadocia (IMSTEC'17), 11 - 13 October 2017
- XXV. **ELECTRONIC PROPERTIES OF CO3O4 NANOCLUSTER FROM DENSITY-FUNCTIONAL CALCULATIONS**  
MUZ İ., KURBAN M.  
International Conference on Material Science and Technology in Cappadocia (IMSTEC'17), 11 - 13 October 2017
- XXVI. **THE STRUCTURE AND ENERGETIC OF ARSENIDE DOPED BORON CLUSTERS (N=1-9)**  
MUZ İ., KURBAN M., Şanlı K.  
International Conference on Material Science and Technology in Cappadocia (IMSTEC'17), 11 - 13 October 2017
- XXVII. **Investigation of Some Physical Features of GaAs Nanoparticles for Solar Cell Applications**  
KURBAN M., GÖKTAŞ F.  
INTERNATIONAL CONFERENCE ON CONDENSED MATTER AND MATERIALS SCIENCE, 11 - 15 October 2017
- XXVIII. **Molecular Dynamics Simulation of Cu55 Magic Cluster on the Graphene Monolayer**  
KURBAN M., Erkoç Ş.  
INTERNATIONAL CONFERENCE ON CONDENSED MATTER AND MATERIALS SCIENCE, 11 - 15 October 2017
- XXIX. **Investigation of geometrical, electronic and spectroscopic properties of Fluorene-9-phenol molecule**  
ÇELİK S., KURBAN M., ÖZKAN KOTİLOĞLU S., TANIŞ E.  
III. International Turkish Congress on Molecular Spectroscopy, Bodrum, Turkey, 26 - 29 August 2017, pp.108
- XXX. **A theoretical study of solvent effects on 2-acetoxybenzoic acid molecule**  
ÇELİK S., TANIŞ E., ÖZKAN KOTİLOĞLU S., KURBAN M.  
III. International Turkish Congress on Molecular Spectroscopy, Bodrum, Turkey, 26 - 29 August 2017, pp.154
- XXXI. **Experimental and Theoretical Study on the Electronic and Optoelectronic Properties of 5,5'-Dibromo-2,2'-bithiophene Organic Material for Photovoltaic Application**  
KURBAN M., GÜNDÜZ B.  
4th International conference on materials and nanotechnology for next generation (MSG2017), Sarajevo, Bosnia And Herzegovina, 28 - 30 June 2017, pp.51
- XXXII. **UV Characterizations of 5-Bromo-2-nitropyridine: Experimental and Theoretical Research**  
KURBAN M., GÜNDÜZ B.

- 4th International conference on materials science and nanotechnology for next generation (MSNG2017), Sarajevo, Bosnia And Herzegovina, 28 - 30 June 2017, pp.52
- XXXIII. **Determination of electronic spectroscopic and optical properties of DCJTb semiconductor by experimental solution technique and theoretical quantum mechanical method**  
GÜNDÜZ B., KURBAN M.  
2nd International Advanced and Functional Materials Technologies (AFMAT), Antalya, Turkey, 20 - 22 October 2016, pp.36
- XXXIV. **Computational and experimental thin film investigations on structure energetics and spectroscopy properties of DCJTb**  
KURBAN M., GÜNDÜZ B.  
2nd International Advanced and Functional Materials Technologies (AFMAT), Antalya, Turkey, 20 - 22 October 2016, pp.31
- XXXV. **Size dependence and segregation phenomena of copper hydride nanoparticles: A molecular dynamics study**  
KURBAN M.  
Turkish Physical Society 32nd International Physics Conference, Bodrum, Turkey, 6 - 09 September 2016
- XXXVI. **A molecular dynamics study on the geometrical and energetics properties of Gallium Arsenide nanoparticles under heat treatment**  
KURBAN M.  
Turkish Physical Society 32nd International Physics Conference, Bodrum, Turkey, 6 - 09 September 2016
- XXXVII. **Core and surface segregation and thermal properties of CdTe<sub>0.5</sub>Se<sub>0.5</sub> ternary nanoparticles**  
KURBAN M.  
12th International Nanoscience and Nanotechnology Conference, Gebze, Turkey, 3 - 05 June 2016, pp.98
- XXXVIII. **Geometrical and energetic properties of 15 atom ternary Cd Zn Te clusters**  
KURBAN M., ERKOÇ Ş.  
9th International Physics Conference of the Balkan Physical Union, İstanbul, Turkey, 24 - 27 August 2015, pp.373
- XXXIX. **CdxZnyTez Nanoparçacıkların Termodinamik Özelliklerinin Moleküler Dinamiği Benzetimi ile İncelenmesi**  
KURBAN M., MALCIOĞLU O. B., ERKOÇ Ş.  
20. YOĞUN MADDE FİZİĞİ ANKARA TOPLANTISI, Ankara, Turkey, 26 December 2014, pp.16
- XL. **Proper Gaussian basis sets for density functional studies of cobalt oxide clusters**  
KURBAN M., ERKOÇ Ş.  
31st international physics congress, Bodrum, Turkey, 21 - 24 July 2014, pp.297
- XLI. **A molecular dynamics study of the heat capacity of CdTe and ZnTe nanoparticles**  
KURBAN M., MALCIOĞLU O. B., ERKOÇ Ş.  
31st international physics congress, Bodrum, Turkey, 21 - 24 July 2014, pp.296
- XLII. **Size dependence and heat capacity of CdZnTe and CdZn nanoparticles: Molecular dynamics simulations**  
KURBAN M., MALCIOĞLU O. B., ERKOÇ Ş.  
31st international physics congress, Bodrum, Turkey, 21 - 24 July 2014, pp.295
- XLIII. **Structural properties of ZnTe and CdTe binary nanorods: Molecular Dynamics Simulations**  
KURBAN M., ERKOÇ Ş.  
30th International Physics Congress, İstanbul, Turkey, 2 - 05 September 2013, pp.371
- XLIV. **Structural and electronic properties of Zn<sub>m</sub>Cd<sub>n</sub>Te<sub>k</sub> clusters: Density functional theory calculations**  
KURBAN M., ERKOÇ Ş.  
9th NANOSCIENCE AND NANOTECHNOLOGY CONFERENCE, Erzurum, Turkey, 24 - 28 June 2013, pp.124
- XLV. **Structural properties of Zn<sub>x</sub>Cd<sub>1-x</sub>Te<sub>0.25</sub> and 0.50 nanorods**  
KURBAN M., ERKOÇ Ş.  
8th NANOSCIENCE AND NANOTECHNOLOGY CONGRESS, Ankara, Turkey, 25 - 29 June 2012, pp.234
- XLVI. **Time Dependent Quantum Study of the H<sub>2</sub>S + F<sub>2</sub> + OH<sub>2</sub> + F<sub>2</sub>P Reaction**

- TUTUK R., KARABULUT E., KURBAN M., GÖKTAŞ F.  
26. ULUSLARARASI FİZİK KONGRESİ, Bodrum, Turkey, 24 - 27 September 2009, pp.339
- XLVII. **Quantum Wave Packet Study of D FO Reaction**  
KURBAN M., KARABULUT E., TUTUK R., GÖKTAŞ F.  
26. ULUSLARARASI FİZİK KONGRESİ, Bodrum, Turkey, 24 - 27 September 2009, pp.316
- XLVIII. **Time Dependent Quantum Dynamics study of Reactive Scattering of the H OF Reaction on the 13A and 13A States**  
KURBAN M., GÖKTAŞ F., KARABULUT E., TUTUK R.  
27 TH INTERNATIONAL PHYSICS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.469
- XLIX. **Quantum Real Wave packet Study of H 2S FO 2 HF 1 O 3P Reaction on the 13A State**  
KURBAN M., KARABULUT E., TUTUK R., GÖKTAŞ F.  
27TH INTERNATINONAL PHYSICS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.468
- L. **Time Dependent Quantum Study of the Reaction of Hydrogen Isotopes and Flouroxide Molecule**  
KURBAN M., KARABULUT E., GÖKTAŞ F.  
27 TH INTERNATIONAL PHYSICS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.470
- LI. **Quantum Wave Packet Study of the HCaCl( v, j) -- HCl ( v, j) Ca Reaction**  
TUTUK R., KARABULUT E., KURBAN M., GÖKTAŞ F.  
27TH INTERNATIONAL PHYSICS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.88
- LII. **Quantum Dynamics Study of H LiF reaction**  
KARABULUT E., KURBAN M., TUTUK R., GÖKTAŞ F.  
27 TH INTERNATIONAL PHYSCIS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.457
- LIII. **Quantum Wave Packet Calculation of Reaction Probabilities Cross Section and Rate Constant for H FO System on the 11A State**  
KURBAN M., GÖKTAŞ F.  
27 TH INTERNATIONAL PHYSICS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.471
- LIV. **Isotope Effects in the XLiF -- XF Li (X = H , D) Reaction**  
KARABULUT E., KURBAN M., TUTUK R., GÖKTAŞ F.  
27 TH INTERNATIONAL PHYSCIS CONGRESS, İstanbul, Turkey, 14 - 17 September 2010, pp.458
- LV. **The Investigation of Photo Dissociation by Time Dependent Quantum Method**  
KURBAN M., KARABULUT E., TUTUK R., GÖKTAŞ F.  
26. ULUSLARARASI FİZİK KONGRESİ, Bodrum, Turkey, 24 - 27 September 2009, pp.317

## Scientific Refereeing

TRANSACTIONS ON ELECTRICAL AND ELECTRONIC MATERIALS, Journal Indexed in ESCI, March 2024  
 COMPUTATIONAL MATERIALS SCIENCE, Journal Indexed in SCI-E, March 2024  
 JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, March 2024  
 LETTERS IN ORGANIC CHEMISTRY, Journal Indexed in SCI-E, February 2024  
 Surfaces and Interfaces, Journal Indexed in SCI-E, February 2024  
 SPECTROCHIMICA ACTA - PART A: MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, Journal Indexed in SCI-E, February 2024  
 MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, Journal Indexed in SCI-E, February 2024  
 MATERIALS TODAY COMMUNICATIONS, Journal Indexed in SCI-E, February 2024  
 COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, February 2024  
 LETTERS IN ORGANIC CHEMISTRY, Journal Indexed in SCI-E, February 2024  
 COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, February 2024  
 JOURNAL OF MOLECULAR LIQUIDS, Journal Indexed in SCI-E, January 2024  
 COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, January 2024  
 PHYSICA B: CONDENSED MATTER, Journal Indexed in SCI-E, January 2024  
 JOURNAL OF MATERIALS SCIENCE, Journal Indexed in SCI-E, January 2024

CHEMISTRYOPEN, Journal Indexed in SCI-E, January 2024  
PHYSICA B: CONDENSED MATTER, Journal Indexed in SCI-E, January 2024  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, December 2023  
MOLECULAR SIMULATION, Journal Indexed in SCI-E, December 2023  
PLASMONICS, Journal Indexed in SCI-E, December 2023  
SILICON, Journal Indexed in SCI-E, December 2023  
MATERIALS CHEMISTRY AND PHYSICS, Journal Indexed in SCI-E, December 2023  
MATERIALS TODAY COMMUNICATIONS, Journal Indexed in SCI-E, December 2023  
GAZI UNIVERSITY JOURNAL OF SCIENCE, National Scientific Refreed Journal, December 2023  
SOLID STATE COMMUNICATIONS, Journal Indexed in SCI-E, November 2023  
PHYSICA B: CONDENSED MATTER, Journal Indexed in SCI-E, November 2023  
MATERIALS CHEMISTRY AND PHYSICS, Journal Indexed in SCI-E, November 2023  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, November 2023  
DISCOVER NANO, Journal Indexed in SCI-E, November 2023  
CHEMICAL PHYSICS, Journal Indexed in SCI-E, October 2023  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, Journal Indexed in SCI-E, October 2023  
INORGANIC CHEMISTRY COMMUNICATION, Journal Indexed in SCI-E, October 2023  
CHEMISTRYSELECT, Journal Indexed in SCI-E, September 2023  
OPTICAL AND QUANTUM ELECTRONICS, Journal Indexed in SCI-E, September 2023  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, Journal Indexed in SCI-E, September 2023  
INDOOR AIR, Journal Indexed in SCI-E, September 2023  
JOURNAL OF AFFECTIVE DISORDERS, Journal Indexed in SCI-E, September 2023  
BMC Chemistry, Journal Indexed in SCI-E, August 2023  
TRANSACTIONS ON ELECTRICAL AND ELECTRONIC MATERIALS, Journal Indexed in ESCI, August 2023  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, Journal Indexed in SCI-E, August 2023  
JOURNAL OF COMPUTATIONAL BIOPHYSICS AND CHEMISTRY, Journal Indexed in SCI-E, August 2023  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, August 2023  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, August 2023  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, August 2023  
PHYSICA B: CONDENSED MATTER, Journal Indexed in SCI-E, August 2023  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, Journal Indexed in SCI-E, July 2023  
MATERIALS TODAY COMMUNICATIONS, Journal Indexed in SCI-E, July 2023  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, June 2023  
JOURNAL OF CLUSTER SCIENCE, Journal Indexed in SCI-E, May 2023  
ARABIAN JOURNAL OF CHEMISTRY, Journal Indexed in SCI-E, May 2023  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, May 2023  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, May 2023  
BIONANOSCIENCE, Journal Indexed in ESCI, May 2023  
OPTICAL AND QUANTUM ELECTRONICS, Journal Indexed in SCI-E, April 2023  
Journal of Magnesium and Alloys, Journal Indexed in SCI-E, March 2023  
INTERNATIONAL JOURNAL OF PHOTOENERGY, Journal Indexed in SCI-E, March 2023  
JOURNAL OF MOLECULAR MODELING, Journal Indexed in SCI-E, March 2023  
MATERIALS TODAY COMMUNICATIONS, Journal Indexed in SCI-E, March 2023  
JOURNAL OF MOLECULAR MODELING, Journal Indexed in SCI-E, March 2023  
SCIENTIFIC REPORTS, Journal Indexed in SCI-E, March 2023  
MATERIALS AND DESIGN, Journal Indexed in SCI-E, February 2023  
PHYSICA SCRIPTA, Journal Indexed in SCI-E, January 2023

## Metrics

Publication: 127

Citation (WoS): 854

Citation (Scopus): 998

H-Index (WoS): 18

H-Index (Scopus): 20