

## Assoc. Prof. SAVAŞ KAYA

### Personal Information

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### Education Information

Doctorate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2013 - 2017

Postgraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2011 - 2013

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2007 - 2011

### Dissertations

Doctorate, Kimyasal sertlik ve elektronegatiflik kavramlarına ilişkin dengelenme ilkelerinin kimyadaki bazı yeni uygulamaları, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2017

Postgraduate, İzoelektronik serilerde kimyasal sertlik ve mutlak elektronegatifliğin incelenmesi, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2013

### Research Areas

Chemistry

### Academic Titles / Tasks

Associate Professor, Sivas Cumhuriyet University, Sağlık Hizmetleri Meslek Yüksekokulu, Eczacılık Bölümü, 2013 - Continues

### Academic and Administrative Experience

Sivas Cumhuriyet Üniversitesi, İmranlı Meslek Yüksekokulu, Mülkiyet Koruma Ve Güvenlik Bölümü, 2013 - Continues

### Courses

Temel Kimya, Associate Degree, 2020 - 2021

Çevre Sağlığı ve Koruma, Associate Degree, 2020 - 2021

Temel Kimya, Associate Degree, 2020 - 2021

İtfaiye Araç ve Malzeme Bilgisi - II, Associate Degree, 2018 - 2019

Yapı ve Elektrik İşlerinde İSG, Associate Degree, 2018 - 2019

Arama Kurtarma Teknikleri, Associate Degree, 2018 - 2019

İş Sağlığı ve Güvenliği Risk Analizi, Associate Degree, 2019 - 2020

Genel Kimya, Associate Degree, 2019 - 2020

İş Kazaları ve Raporlama, Associate Degree, 2018 - 2019  
Toksikoloji ve Zehirlenmeler, Associate Degree, 2019 - 2020  
Temel Elektrik ve Elektronik Bilgisi, Associate Degree, 2018 - 2019  
Kimyasallar ve Tehlikeleri, Associate Degree, 2018 - 2019  
İtfaiye Araç ve Malzeme Bilgisi - I, Associate Degree, 2018 - 2019  
Toksikoloji ve Zehirlenmeler, Associate Degree, 2016 - 2017, 2017 - 2018  
Taşıma ve Depolama, Associate Degree, 2017 - 2018  
Uyarı İşaretleri ve Levha Standartları, Associate Degree, 2018 - 2019  
Kimyasallar ve Tehlikeleri, Associate Degree, 2017 - 2018  
Genel Kimya, Associate Degree, 2016 - 2017, 2017 - 2018  
Taşıma ve Depolama, Associate Degree, 2016 - 2017, 2017 - 2018  
Matematik - I, Associate Degree, 2016 - 2017  
Matematik 2, Associate Degree, 2016 - 2017  
Matematik 1, Associate Degree, 2016 - 2017  
Matematik - II, Associate Degree, 2016 - 2017  
İlk Yardım ve Sağlık Bilgisi, Associate Degree, 2016 - 2017  
İngilizce - I, Associate Degree, 2016 - 2017  
İngilizce 1, Associate Degree, 2016 - 2017  
Bilgisayar - I, Associate Degree, 2016 - 2017  
İngilizce - II, Associate Degree, 2015 - 2016  
Atatürk İlkeleri ve İnkılap Tarihi - I, Associate Degree, 2014 - 2015  
Ticari Matematik, Associate Degree, 2013 - 2014  
Bilgisayarlı Muhasebe, Associate Degree, 2013 - 2014

## Jury Memberships

Competition, TÜBİTAK - 2204 - B ORTAOKUL ÖĞRENCİLERİ ARAŞTIRMA PROJELERİ YARIŞMASI, TÜBİTAK, October, 2020

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

- I. **Molecular dynamic simulations and computational DFT of adsorption performances of malachite green on the metal fluorides in aqueous medium**  
Boumya W., Khnifira M., Abdennouri M., KAYA S., Achak M., Barka N.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1270, 2022 (Peer-Reviewed Journal)
- II. **Effect of electron donors on the photophysical and theoretical properties of BODIPY dyes based on tetrazolo [1,5-a]quinoline**  
Arslana B. S. , Derin Y., Misir B. A. , KAYA S., ŞİŞMAN İ., TUTAR A., NEBİOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1267, 2022 (Peer-Reviewed Journal)
- III. **Experimental, DFT and MC simulation analysis of Vicia Sativa weed aerial extract as sustainable and eco-benign corrosion inhibitor for mild steel in acidic environment**  
Thakur A., KAYA S., Abousalem A. S. , Kumar A.  
SUSTAINABLE CHEMISTRY AND PHARMACY, vol.29, 2022 (Peer-Reviewed Journal)
- IV. **Adsorption study of N (-benzo[d]thiazol-2-yl)-1-(thiophene-2-yl) methanimine at mild steel/aqueous H<sub>2</sub>SO<sub>4</sub> interface**  
Singh A. K. , Singh M., Thakur S., Pani B., KAYA S., EL Ibrahim B., Marzouki R.  
SURFACES AND INTERFACES, vol.33, 2022 (Peer-Reviewed Journal)
- V. **Combined experimental and theoretical analyses on design, synthesis, characterization, and in vitro cytotoxic activity evaluation of some novel imino derivatives containing pyrazolone ring**

Basaran E., ÇAKMAK R., AKKOÇ S., KAYA S.

JOURNAL OF MOLECULAR STRUCTURE, vol.1265, 2022 (Peer-Reviewed Journal)

- VI. **Insights into the role of nanotechnology on the performance of biofuel cells and the production of viable biofuels: A review**  
Assad H., KAYA S., Kumar P. S., Vo D. N., Sharma A., Kumar A.  
FUEL, vol.323, 2022 (Peer-Reviewed Journal)
- VII. **Insight of development of two cured epoxy polymer composite coatings as highly protective efficiency for carbon steel in sodium chloride solution: DFT, RDF, FFV and MD approaches**  
Hsissou R., Azogagh M., Benhiba F., Echihi S., Galai M., Shaim A., Bahaj H., Briche S., KAYA S., Serdaroglu G., et al.  
JOURNAL OF MOLECULAR LIQUIDS, vol.360, 2022 (Peer-Reviewed Journal)
- VIII. **Effect of Hemp Fiber Addition on Mechanical Properties of Acrylic Resin: Coupled Experimental and Theoretical Study**  
BOLAYIR G., SOYGUN K., KILIÇ AVŞAR M., BOZTUĞ A., KAYA S., Katin K. P.  
FIBERS AND POLYMERS, vol.23, no.8, pp.2271-2278, 2022 (Peer-Reviewed Journal)
- IX. **An investigation on the synthesis, characterization and anti-corrosion properties of choline based ionic liquids as novel and environmentally friendly inhibitors for mild steel corrosion in 5% HCl**  
Mobin M., Aslam R., Salim R., KAYA S.  
JOURNAL OF COLLOID AND INTERFACE SCIENCE, vol.620, pp.293-312, 2022 (Peer-Reviewed Journal)
- X. **Designing new donors organic compounds with IDIC core for photovoltaic application**  
Nebbach D., Agda F., Lakhlifi T., Ajana M. A., Kaya S., Siddique F., Lgaz H., Bouachrine M.  
OPTIK, vol.262, 2022 (Peer-Reviewed Journal)
- XI. **Handling Keywords: MXene Nanomaterial Hazardous pollutant Adsorption Environmental remediation**  
Assad H., Fatma I., Kumar A., KAYA S., Vo D. N., Al-Gheethi A., Sharma A.  
CHEMOSPHERE, vol.298, 2022 (Peer-Reviewed Journal)
- XII. **Experimental and density functional theoretical modeling of triazole pesticides extraction by Ti2C nanosheets as a sorbent in dispersive solid phase extraction method before HPLC-MS/MS analysis**  
Marzi Khosrowshahi E., Afshar Mogaddam M. R., Javadzadeh Y., ALTUNAY N., Tuzen M., KAYA S., Ghalkhani M., Farajzadeh M. A., Nemati M.  
Microchemical Journal, vol.178, 2022 (Peer-Reviewed Journal)
- XIII. **Crystal chemistry, DFT calculation and optical properties of the double perovskite stannate Sr<sub>2</sub>Sn<sub>0.8</sub>In<sub>0.8</sub>W<sub>0.4</sub>O<sub>6</sub>**  
Belgacem B., Maslov M. M., KAYA S., Ali I. H., Ben Hassen B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1259, 2022 (Peer-Reviewed Journal)
- XIV. **Quantum chemical and molecular dynamics simulation approach to investigate adsorption behaviour of organic azo dyes on TiO<sub>2</sub> and ZnO surfaces**  
Mandal S., Zamindar S., Sarkar S., Murmu M., Guo L., KAYA S., Hirani H., Banerjee P.  
JOURNAL OF ADHESION SCIENCE AND TECHNOLOGY, 2022 (Peer-Reviewed Journal)
- XV. **New mixed-ligand iron(III) complexes containing thiocarbohydrazones: Preparation, characterization, and chemical reactivity analysis through theoretical calculations**  
KAYA Y., ERÇAĞ A., KAYA S., Katin K. P., ATILLA D.  
APPLIED ORGANOMETALLIC CHEMISTRY, 2022 (Peer-Reviewed Journal)
- XVI. **On the Prediction of Lattice Energy with the Fukui Potential: Some Supports on Hardness Maximization in Inorganic Solids**  
KAYA S., Robles-Navarro A., Mejia E., Gomez T., Cardenas C.  
JOURNAL OF PHYSICAL CHEMISTRY A, 2022 (Peer-Reviewed Journal)
- XVII. **Removal of erythrosine B dye from wastewater using chitosan boric acid composite material: Experimental and density functional theory findings**  
Cetinkaya H. F., SARIOĞLU CEBECİ M., KAYA S., Jalbani N. S., Maslov M. M., Marzouki R.  
JOURNAL OF PHYSICAL ORGANIC CHEMISTRY, 2022 (Peer-Reviewed Journal)
- XVIII. **Experimental and density functional theory studies during a new solid phase extraction of phenolic**

**compounds from wastewater samples prior to GC–MS determination**

Farajzadeh M. A. , Nemati M., ALTUNAY N., Tuzen M., KAYA S., Kheradmand F., Afshar Mogaddam M. R.  
Microchemical Journal, vol.177, 2022 (Peer-Reviewed Journal)

- XIX. **Computational and experimental studies on the corrosion inhibition performance of an aerial extract of Cnicus Benedictus weed on the acidic corrosion of mild steel**  
Thakur A., KAYA S., Abousalem A. S. , Sharma S., Ganjoo R., Assad H., Kumar A.  
PROCESS SAFETY AND ENVIRONMENTAL PROTECTION, vol.161, pp.801-818, 2022 (Peer-Reviewed Journal)
- XX. **An insight about the interaction of Aryl Benzothiazoles with mild steel surface in aqueous HCl solution**  
Sheetal S., Sengupta S., Singh M., Thakur S., Pani B., Banerjee P., KAYA S., Singh A. K.  
JOURNAL OF MOLECULAR LIQUIDS, vol.354, 2022 (Peer-Reviewed Journal)
- XXI. **Fluorinated carbon and boron nitride fullerenes for drug Delivery: Computational study of structure and adsorption**  
Kalika E. B. , Katin K. P. , Kochaev A., KAYA S., ELİK M., Maslov M. M.  
JOURNAL OF MOLECULAR LIQUIDS, vol.353, 2022 (Peer-Reviewed Journal)
- XXII. **Theoretical and experimental insights about the adsorption of uranyl ion on a new designed Vermiculite-Polymer composite**  
Şimşek S., Kaya S., Mine Şenol Z. M. , Ulusoy H. İ. , Katin K., Özer A., Altunay N., Brahmia A.  
Journal of Molecular Liquids, vol.352, 2022 (Peer-Reviewed Journal)
- XXIII. **One-Pot Hydrothermal Synthesized Nitrogen and Sulfur Codoped Carbon Dots for Acid Corrosion Inhibition of Q235 Steel br**  
Guo L., Zhu M., He Z., Zhang R., KAYA S., Lin Y., Saji V. S.  
LANGMUIR, vol.38, no.13, pp.3984-3992, 2022 (Peer-Reviewed Journal)
- XXIV. **A comprehensive and current review on the role of flavonoids in lung cancer–Experimental and theoretical approaches**  
BERK Ş., KAYA S., Akkol E. K. , BARDAKCI H.  
Phytomedicine, vol.98, 2022 (Peer-Reviewed Journal)
- XXV. **Natural corrosion inhibitor of renewable eco-waste for SS-410 in sulfuric acid medium: adsorption, electrochemical, and computational studies**  
Prasad D., Singh R., KAYA S., el Ibrahim B.  
JOURNAL OF MOLECULAR LIQUIDS, vol.351, 2022 (Peer-Reviewed Journal)
- XXVI. **Can van der Waals constants be used in the chemical reactivity analysis? A new approach as a support to minimum magnetizability principle**  
KAYA S., ŞİMŞEK S.  
JOURNAL OF PHYSICAL ORGANIC CHEMISTRY, 2022 (Peer-Reviewed Journal)
- XXVII. **Synthesis, spectral characterization, chemical reactivity and anticancer behaviors of some novel hydrazone derivatives: Experimental and theoretical insights**  
ÇAKMAK R., Basaran E., KAYA S., ERKAN S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1253, 2022 (Peer-Reviewed Journal)
- XXVIII. **A benzimidazolium salt as effective corrosion inhibitor against the corrosion of mild steel in acidic medium: experimental and theoretical studies**  
ŞAHİN N., KAYA S., Aydin O., Katin K. P. , Chaouiki A., GÜRBÜZ N., ÖZDEMİR İ., FARSAK M.  
JOURNAL OF ADHESION SCIENCE AND TECHNOLOGY, 2022 (Peer-Reviewed Journal)
- XXIX. **Kaya's composite descriptor and Maximum Composite Hardness Rule for chemical reactions**  
KAYA S., ÖZBAKIR İŞİN D., KARAKUŞ N.  
JOURNAL OF THE INDIAN CHEMICAL SOCIETY, vol.99, no.3, 2022 (Peer-Reviewed Journal)
- XXX. **Novel gossypol-indole modification as a green corrosion inhibitor for low-carbon steel in aggressive alkaline-saline solution**  
Berdimurodov E., Kholikov A., Akbarov K., Guo L., KAYA S., Katin K. P. , Verma D. K. , Rbaa M., Dagdag O., Haldhar R.  
COLLOIDS AND SURFACES A-PHYSCOCHEMICAL AND ENGINEERING ASPECTS, vol.637, 2022 (Peer-Reviewed Journal)

- XXXI. **Development of dispersive solid-liquid extraction method based on organic polymers followed by deep eutectic solvents elution; application in extraction of some pesticides from milk samples prior to their determination by HPLC-MS/MS**  
Nemati M., TÜZEN M., Farazajdeh M. A. , KAYA S., Mogaddam M. R. A.  
ANALYTICA CHIMICA ACTA, vol.1199, 2022 (Peer-Reviewed Journal)
- XXXII. **Development of QSAR-based (MLR/ANN) predictive models for effective design of pyridazine corrosion inhibitors**  
Quadri T. W. , Olasunkanmi L. O. , Akpan E. D. , Fayemi O. E. , Lee H., Lgaz H., Verma C., Guo L., KAYA S., Ebenso E. E.  
MATERIALS TODAY COMMUNICATIONS, vol.30, 2022 (Peer-Reviewed Journal)
- XXXIII. **Suppressing inhibitory compounds by nanomaterials for highly efficient biofuel production: A review**  
Thakur A., Kumar A., KAYA S., Vo D. N. , Sharma A.  
FUEL, vol.312, 2022 (Peer-Reviewed Journal)
- XXXIV. **Mathematical modeling studies for the adsorptive removal of ciprofloxacin drug from water samples using functionalized silica resin**  
Junejo R., Jalbani N. S. , KAYA S., SERDAROĞLU G., ELİK M.  
CHEMICAL PAPERS, 2022 (Peer-Reviewed Journal)
- XXXV. **Non-fullerene acceptor IDIC based on indacinodithiophene used as an electron donor for organic solar cells: A computational study**  
Nebbach D., Agda F., KAYA S., Siddique F., Lakhlifi T., Ajana M. A. , Bouachrine M.  
JOURNAL OF MOLECULAR LIQUIDS, vol.348, 2022 (Peer-Reviewed Journal)
- XXXVI. **Experimental and DFT Modeling Studies for the Adsorptive Removal of Reactive Dyes from Wastewater**  
Junejo R., Shams Jalbani N., KAYA S., SERDAROĞLU G., ŞİMŞEK S., Memon S.  
SEPARATION SCIENCE AND TECHNOLOGY, vol.57, no.3, pp.339-353, 2022 (Peer-Reviewed Journal)
- XXXVII. **An experimental and theoretical approach to electrochemical sensing of environmentally hazardous dihydroxy benzene isomers at polysorbate modified carbon paste electrode**  
Ganesh P., Kim S., KAYA S., Salim R.  
SCIENTIFIC REPORTS, vol.12, no.1, 2022 (Peer-Reviewed Journal)
- XXXVIII. **Ab Initio Insight into the Interaction of Metal-Decorated Fluorinated Carbon Fullerenes with Anti-COVID Drugs**  
Katin K. P. , Kochaev A. I. , KAYA S., El-Hajjaji F., Maslov M. M.  
INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES, vol.23, no.4, 2022 (Peer-Reviewed Journal)
- XXXIX. **Novel glycoluril pharmaceutically active compound as a green corrosion inhibitor for the oil and gas industry**  
Berdimurodov E., Kholikov A., Akbarov K., Guo L., KAYA S., Verma D. K. , Rbaa M., Dagdag O.  
JOURNAL OF ELECTROANALYTICAL CHEMISTRY, vol.907, 2022 (Peer-Reviewed Journal)
- XL. **Phenylamine/Amide Grafted in Silica as Sensing Nanocomposites for the Removal of Carbamazepine: A DFT Approach**  
Algarra M., Jodeh S., Aqel I., Hanbali G., Radi S., Tighadouini S., Alkowni R., Soto J., Samhan S., KAYA S., et al.  
CHEMOSENSORS, vol.10, no.2, 2022 (Peer-Reviewed Journal)
- XLI. **Recent Innovations in Nano Container-Based Self-Healing Coatings in the Construction Industry**  
Thakur A., KAYA S., Kumar A.  
CURRENT NANOSCIENCE, vol.18, no.2, pp.203-216, 2022 (Peer-Reviewed Journal)
- XLII. **Equilibrium, thermodynamic, and kinetic modeling studies for the adsorptive removal of oxyanions from water**  
Junejo R., Shams Jalbani N., KAYA S., SERDAROĞLU G., ELİK M., Memon S.  
SEPARATION SCIENCE AND TECHNOLOGY, 2021 (Peer-Reviewed Journal)
- XLIII. **Spectral studies and quantum chemical ab initio calculations for Copper(II) complexes of two heterocyclic aroylhydrazones**  
Sheeja S. R. , Mangalam N. A. , Sithambaresan M., Kurup M. R. P. , Kaya S., Serdaroğlu G.

JOURNAL OF MOLECULAR STRUCTURE, vol.1245, 2021 (Peer-Reviewed Journal)

- XLIV. **Performance of curing epoxy resin as potential anticorrosive coating for carbon steel in 3.5% NaCl medium: Combining experimental and computational approaches**  
Hsissou R, Benhiba F, Echihi S, Benzidia B, Cherrouf S, Haldhar R, Alvi P. A. , KAYA S, SERDAROĞLU G, Zarrouk A.  
CHEMICAL PHYSICS LETTERS, vol.783, 2021 (Peer-Reviewed Journal)
- XLV. **Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives**  
Kaya Y., Erçağ A., Serdaroglu G., Kaya S., Grillo I. B. , Rocha G. B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1244, 2021 (Peer-Reviewed Journal)
- XLVI. **Inhibition effect of newly synthesized benzoxanthonederivative on hydrogen evolution and Q235 steelcorrosion in 15% HCl under hydrodynamic condition: Combination of experimental, surface and computational study**  
Singh A, Bedi P, Ansari K. R. , Pramanik T, Chaudhary D., Santra S., Alanazi A. K. , Das S., Quraishi M. A. , Lin Y., et al.  
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.46, no.76, pp.37995-38007, 2021 (Peer-Reviewed Journal)
- XLVII. **Experimental and theoretical investigation on the inhibition performance of disulfide derivatives on cobalt corrosion in alkaline medium**  
Ma T, Tan B, Guo L, Wang W, Li W, Ji J, Yan M, KAYA S.  
JOURNAL OF MOLECULAR LIQUIDS, vol.341, 2021 (Peer-Reviewed Journal)
- XLVIII. **Novel bromide-cucurbit[7]uril supramolecular ionic liquid as a green corrosion inhibitor for the oil and gas industry**  
Berdimurodov E, Kholikov A, Akbarov K, Guo L, KAYA S, Katin K. P. , Verma D. K. , Rbaa M, Dagdag O, Haldhar R.  
JOURNAL OF ELECTROANALYTICAL CHEMISTRY, vol.901, 2021 (Peer-Reviewed Journal)
- XLIX. **Multidimensional insights into the corrosion inhibition of potassium oleate on Cu in alkaline medium: A combined Experimental and theoretical investigation**  
Ma T, Tan B, Guo L, KAYA S, Kao Z, Zhang S, Wang R, Zeng N, He Y.  
MATERIALS SCIENCE AND ENGINEERING B-ADVANCED FUNCTIONAL SOLID-STATE MATERIALS, vol.272, 2021 (Peer-Reviewed Journal)
- L. **Papaver somniferum as an efficient corrosion inhibitor for iron alloy in acidic condition: DFT, MC simulation, LCMS and electrochemical studies**  
Haldhar R, Kim S, Prasad D, Bedair M. A. , Bahadur I, KAYA S, Dagdag O, Guo L.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1242, 2021 (Peer-Reviewed Journal)
- LI. **Electrochemical investigations and theoretical studies of biocompatible niacin-modified carbon paste electrode interface for electrochemical sensing of folic acid**  
Ganesh P, Kim S, Choi D, KAYA S, SERDAROĞLU G, Shimoga G, Shin E, Lee S.  
JOURNAL OF ANALYTICAL SCIENCE AND TECHNOLOGY, vol.12, no.1, 2021 (Peer-Reviewed Journal)
- LII. **Molecular modelling of compounds used for corrosion inhibition studies: a review**  
Ebenso E. E. , Verma C, Olasunkanmi L. O. , Akpan E. D. , Verma D. K. , Lgaz H, Guo L, KAYA S, Quraishi M. A.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.23, pp.19987-20027, 2021 (Peer-Reviewed Journal)
- LIII. **Novel antioxidant quinoxaline derivative: Synthesis, crystal structure, theoretical studies, antidiabetic activity and molecular docking study**  
Missioui M, Mortada S, Guerrab W, Serdaroglu G, KAYA S, Mague J. T. , Essassi E. M. , Faouzi M. E. A. , Ramli Y.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1239, 2021 (Peer-Reviewed Journal)
- LIV. **Decyltriphenylphosphonium bromide containing hydrophobic alkyl-chain as a potential corrosion inhibitor for mild steel in sulfuric acid: Theoretical and experimental studies**  
Goyal M, Vashisht H, Alrefae S. H. , Jain R, Kumar S, KAYA S, Guo L, Verma C.  
JOURNAL OF MOLECULAR LIQUIDS, vol.336, 2021 (Peer-Reviewed Journal)
- LV. **Chemical characterization and evaluation of the neuroprotective potential of Indigofera sessiliflora through in-silico studies and behavioral tests in scopolamine-induced memory compromised rats**  
Haider M. S. , Ashraf W., Javaid S, Rasool M. F. , Rahman H. M. A. , Saleem H, Anjum S. M. M. , Siddique F, Morales-

Bayuelo A., KAYA S., et al.

SAUDI JOURNAL OF BIOLOGICAL SCIENCES, vol.28, no.8, pp.4384-4398, 2021 (Peer-Reviewed Journal)

- LVI. **Investigation of plant waste as a renewable biomass source to develop efficient, economical and eco-friendly corrosion inhibitor**  
Haldhar R., Prasad D., Bahadur I., Dagdag O., KAYA S., Verma D. K., Kim S.  
JOURNAL OF MOLECULAR LIQUIDS, vol.335, 2021 (Peer-Reviewed Journal)
- LVII. **Quantum chemical studies and electrochemical investigations of pyrogallol red modified carbon paste electrode fabrication for sensor application**  
Ganesh P., Shimoga G., Kim S., Lee S., KAYA S., Salim R.  
MICROCHEMICAL JOURNAL, vol.167, 2021 (Peer-Reviewed Journal)
- LVIII. **Corrosion inhibition, surface adsorption and computational studies of Swertia chirata extract: A sustainable and green approach**  
Haldhar R., Prasad D., Nguyen L. T. D., KAYA S., Bahadur I., Dagdag O., Kim S.  
MATERIALS CHEMISTRY AND PHYSICS, vol.267, 2021 (Peer-Reviewed Journal)
- LIX. **Thermo-magnetic properties of the screened Kratzer potential with spatially varying mass under the influence of Aharonov-Bohm(AB) and position-dependent magnetic fields**  
Edet C. O., Ikot A. N., Onyeaju M. C., Okorie U. S., Rampho G. J., Lekala M. L., KAYA S.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.131, 2021 (Peer-Reviewed Journal)
- LX. **Zeolite/Cellulose Acetate (ZCA) in Blend Fiber for Adsorption of Erythromycin Residue From Pharmaceutical Wastewater: Experimental and Theoretical Study**  
Jodeh S., Erman I., Hamed O., Massad Y., Hanbali G., Samhan S., Dagdag O., KAYA S., SERDAROĞLU G.  
FRONTIERS IN CHEMISTRY, vol.9, 2021 (Peer-Reviewed Journal)
- LXI. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2 '-disulfanediybis(tetrahydro-4H-cyclopenta[d][1,3,2]dioxaphosphole-2-sulfide)**  
Mkadmh A. M., Safi Z. S., Elkhaldy A. A., Staples R. J., KAYA S., SERDAROĞLU G.  
JOURNAL OF COMPUTATIONAL CHEMISTRY, 2021 (Peer-Reviewed Journal)
- LXII. **Probing of Neural Networks as a Bridge from Ab Initio Relevant Characteristics to Differential Scanning Calorimetry Measurements of High-Energy Compounds**  
Bondarev N., Katin K. P., Merinov V. B., Kochaev A., KAYA S., Maslov M. M.  
PHYSICA STATUS SOLIDI-RAPID RESEARCH LETTERS, 2021 (Peer-Reviewed Journal)
- LXIII. **Two empirical formulae for estimating standard entropy of inorganic ionic solids and a possible connection between two associated electronic structure principles**  
KAYA S., Chattaraj P. K., SERDAROĞLU G.  
POLYHEDRON, vol.202, 2021 (Peer-Reviewed Journal)
- LXIV. **Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries**  
Zulueta Y. A., Mut R., KAYA S., Dawson J. A., Minh Tho Nguyen M. T. N.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.125, no.27, pp.14947-14956, 2021 (Peer-Reviewed Journal)
- LXV. **Quantum Chemical Studies and Electrochemical Investigations of Polymerized Brilliant Blue-Modified Carbon Paste Electrode for In Vitro Sensing of Pharmaceutical Samples**  
Ganesh P., Kim S., KAYA S., Salim R., Shimoga G., Lee S.  
CHEMOSENSORS, vol.9, no.6, 2021 (Peer-Reviewed Journal)
- LXVI. **Adsorption of Eriochrome Black T on the chitin surface: Experimental study, DFT calculations and molecular dynamics simulation**  
Boumya W., Khnifira M., Machrouhi A., Abdennouri M., Sadiq M., Achak M., SERDAROĞLU G., KAYA S., ŞİMŞEK S., Barka N.  
Journal of Molecular Liquids, vol.331, 2021 (Peer-Reviewed Journal)
- LXVII. **Sour corrosion of C1018 carbon steel and its inhibition by 1-benzylimidazole: electrochemical, SEM, FTIR and computational assessment**  
Onyeachu I. B., Njoku D., Kaya S., El Ibrahim B., Nnadozie C. F.  
JOURNAL OF ADHESION SCIENCE AND TECHNOLOGY, 2021 (Peer-Reviewed Journal)
- LXVIII. **Investigations of Hg(II) analysis in real samples via computational chemistry, experimental design,**

**and green microextraction approach**

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- CXLVI. **Theoretical modeling and molecular level insights into the corrosion inhibition activity of 2-amino-1,3,4-thiadiazole and its 5-alkyl derivatives**  
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- CXLVIII. **Quantum chemical and molecular dynamics simulation studies on inhibition performances of some thiazole and thiadiazole derivatives against corrosion of iron**  
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- CXLIX. **Density Functional Theory (DFT) modeling and Monte Carlo simulation assessment of inhibition performance of some carbohydrazide Schiff bases for steel corrosion**  
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- CL. **Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT and Monte Carlo simulation approaches**  
Obot I. B. , KAYA S., KAYA C., TÜZÜN B.  
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- CLI. **Reply to the "Comment on "A new equation based on ionization energies and electron affinities of atoms for calculating of group electronegativity" by S. Kaya and C. Kaya [Comput. Theoret. Chem. 1052 (2015) 42-46]"**  
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COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1083, pp.75-76, 2016 (Peer-Reviewed Journal)
- CLII. **The nucleophilicity equalization principle and new algorithms for the evaluation of molecular nucleophilicity**  
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- CLIII. **Maximum hardness and minimum polarizability principles through lattice energies of ionic compounds**  
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- CLVII. **A Simple Method for the Calculation of Lattice Energies of Inorganic Ionic Crystals Based on the Chemical Hardness**  
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## Articles Published in Other Journals

- I. **Corrosion behaviour of new oxo-pyrimidine derivatives on mild steel in acidic media: Experimental, surface characterization, theoretical, and Monte Carlo studies**  
Ferigita K. S. M., AlFalah M. G. K., SARAÇOĞLU M., KÖKBUDAK Z., KAYA S., Alaghani M. O. A., KANDEMİRLİ F.  
APPLIED SURFACE SCIENCE ADVANCES, vol.7, 2022 (Peer-Reviewed Journal)
- II. **New and Green Corrosion Inhibitor Based on New Imidazole Derivate for Carbon Steel in 1 M HCl Medium: Experimental and Theoretical Analyses**  
Berdimurodov E., Kholikov A., Akbarov K., Guo L., KAYA S., Verma D. K., Rbaa M., Dagdag O.  
INTERNATIONAL JOURNAL OF ENGINEERING RESEARCH IN AFRICA, vol.58, pp.11-44, 2022 (Peer-Reviewed Journal)
- III. **Crystal structure and Hirshfeld surface analysis of 2-(2-oxo-3-phenyl-1,2,3,8a-tetrahydroquinoxalin-1-yl)ethyl acetate**  
Abad N., El Ghayati L., Mubengayi C. K., Essassi E. M., KAYA S., Mague J. T., Ramli Y.  
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- IV. **Corrosion inhibition, surface adsorption and computational studies of Momordica charantia extract: a sustainable and green approach**  
Haldhar R., Prasad D., Kamboj D., KAYA S., Dagdag O., Guo L.  
SN APPLIED SCIENCES, vol.3, no.1, 2021 (Peer-Reviewed Journal)
- V. **All-nitrogen cages and molecular crystals: Topological rules, stability, and pyrolysis paths**  
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Computation, vol.8, no.4, pp.1-13, 2020 (Peer-Reviewed Journal)
- VI. **Anti-corrosion Properties of 2-Phenyl-4(3H)-quinazolinone-Substituted Compounds: Electrochemical, Quantum Chemical, Monte Carlo, and Molecular Dynamic Simulation Investigation**

- Kacimi Y. E., Tourir R., Alaoui K., KAYA S., Abousalem A. S., Ouakki M., Touhami M. E.  
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- VII. **New triazepine carboxylate derivatives: correlation between corrosion inhibition property and chemical structure**  
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INTERNATIONAL JOURNAL OF INDUSTRIAL CHEMISTRY, vol.11, no.1, pp.23-42, 2020 (Peer-Reviewed Journal)
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- IX. **Electrochemical and Computational Studies of Some Triazepine Carboxylate Compounds as Acid Corrosion Inhibitors for Mild Steel**  
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- X. **Lattice Energies for Groups 1 and 2 Halides from Absolute Hardness**  
FERNANDES DE FARIAS R., KAYA S.  
Cumhuriyet Science Journal, pp.192-195, 2018 (Peer-Reviewed Journal)
- XI. **Experimental and MDS studies of corrosion inhibition of carbon steel by saccharinate sodium**  
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- XII. **Lattice Energies from Hydration Enthalpies: Some acid-base and Structural Considerations**  
KAYA S., DE FARIAS R. F.  
International Journal of Advanced Engineering Research and Science, vol.5, no.8, pp.317-323, 2018 (Peer-Reviewed Journal)
- XIII. **Corrosion inhibition studies for mild steel in 5.0 M HCl by substituted phenyltetrazole**  
El Kacimi Y., Azaroual M. A., Tourir R., Galai M., Alaoui K., Sfaira M., Touhami M. E., Kaya S.  
EURO-MEDITERRANEAN JOURNAL FOR ENVIRONMENTAL INTEGRATION, vol.2, no.1, 2017 (Peer-Reviewed Journal)
- XIV. **Conceptual Density Functional Theoretical Investigation of the Corrosion Inhibition Efficiencies of Some Molecules Containing Mercapto (-SH) Group**  
KAYA S., TÜZÜN B., KAYA C.  
Current Physical Chemistry, vol.7, no.2, pp.147-153, 2017 (Peer-Reviewed Journal)
- XV. **Effect of Molecular Hardness on Ionic Characters, Bond Lengths, Bond Force Constants and Melting Points of Alkali Halides**  
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- XVI. **Validation of the Charge Equalization Principles during the Formation of Small Molecules**  
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- XVII. **Theoretical Investigation of Corrosion Inhibition of Iron Metal by Some Benzothiazole Derivatives: A Monte Carlo Study**  
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- XVIII. **Comments on Electronegativity Equalization with Pauling Units**  
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- XIX. **A Useful Method for the Prediction of Molecular Electrophilicity and Nucleophilicity**  
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- XX. **Derivation of ionization energy and electron affinity equations using chemical hardness and absolute electronegativity in isoelectronic series**  
KAYA S., KAYA C.  
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- XXI. **Investigation of relationship with electron configuration of chemical hardness, absolute electronegativity and electrophilicity**  
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- XXII. **EFFECT OF SOME ELECTRON DONOR AND ELECTRON ACCEPTOR GROUPS ON STABILITY OF COMPLEXES ACCORDING TO THE PRINCIPLE OF HSAB**  
KAYA S., ERKAN KARİPER S., ÜNGÖRDÜ A.  
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- XXIII. **EFFECT OF SOME ELECTRON DONOR AND ELECTRON ACCEPTOR GROUPS ON STABILITY OF COMPLEXES ACCORDING TO THE PRINCIPLE OF HSAB**  
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JOURNAL OF NEW RESULTS IN SCIENCE, pp.82-89, 2014 (Peer-Reviewed Journal)

## **Books & Book Chapters**

- I. **New Challenges and Industrial Applications for Corrosion Prevention and Control**  
Kaya S. (Editor)  
igi-global, New York, 2020
- II. **Phthalonitrile Derivatives Containing Different Heterocyclic Groups as New Corrosion Inhibitors for Iron(110) Surface**  
Yabaş E., Guo L., Safi Z. S., Kaya S.  
in: Research Methodologies and Practical Applications of Chemistry, L. Pogliani, A. K. Haghi, N. Islam, Editor, CRC, New York, Florida, pp.71-89, 2020
- III. **CONCEPTUAL DENSITY FUNCTIONAL THEORY AND ITS APPLICATIONS IN THE CHEMICAL DOMAIN**  
Kaya S. (Editor)  
CRC, New York, New Jersey, 2018
- IV. **Chemical Equalization Principles and Their New Applications**  
KAYA S., KAYA C., OBOT I. B.  
in: Conceptual Density Functional Theory and Its Application in the Chemical Domain, Islam Nazmul, Kaya Savaş, Editor, Apple Academic Press, pp.90-144, 2018
- V. **Conceptual Density Functional Theory and Its Application to Corrosion Inhibition Studies**  
OBOT I. B., KAYA S., KAYA C.  
in: Conceptual Density Functional Theory and Its Applications in the Chemical Domain, Islam Nazmul, Kaya Savaş, Editor, Apple Academic Press, pp.196-216, 2018
- VI. **Ionization Energies of Atoms of 103 Elements of Periodic Table Using Semiempirical and DFT Methods**  
ISLAM N., KAYA S., GHOSH D. C.  
in: Conceptual Density Functional Theory and Its Application in the Chemical Domain, Islam Nazmul, Kaya Savaş, Editor, Apple Academic Press, pp.344-360, 2018

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

- I. **Evaluation of Anticancer, Antimicrobial, Antibiofilm Activity and Molecular Docking Study of Ethanol Extracts of Abies Cilicia (Antoine & Kotschy) Carrière) Resin**  
TAŞ A., GÜÇLÜ G., DİNÇER E., UÇAR SÖZMEN E., DURAL E., KAYA S., SİLİĞ Y.

5 th International Conference on Physical Chemistry & Functional Materials, Sivas, Turkey, 23 June 2022

- II. **A THEORETICAL AND COMPUTATIONAL INSIGHT ON THE TOXICITY OF THE ORGANIC CHEMICALS**  
SERDAROĞLU G., KAYA S.  
The Third Edition of The International Congress On Water And Environment Studies, Morocco, Morocco, 10 December 2020
- III. **The substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indol-3-yl)methanol: Spectroscopic and electronic investigation**  
SERDAROĞLU G., KAYA S.  
International Virtual Conference on Materials and Environmental Science, Morocco, 18 November 2020
- IV. **Electrochemical and theoretical study of the behaviour of a Carbon steel in HCl medium by some triazole type compounds**  
Merimi İ., B H., Merimi C., SZUMIATA T., SERDAROĞLU G., KAYA S.  
4th Edition of the International Virtual Conference on Materials & Environmental Science, Morocco, Morocco, 18 November 2020
- V. **The substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indole-3-yl)methanol: Spectroscopic and electronic investigation**  
SERDAROĞLU G., KAYA S.  
4th Edition of the International Virtual Conference on Materials & Environmental Science, Morocco, Morocco, 18 - 27 November 2020
- VI. **The metal chelation effect on the chemical reactivity of the (E)-2-(2-(pyridin-2-ylmethylene)hydrazineyl) phenol: Theoretical and computational investigation**  
Kaya S., Serdaroglu G., Merimi İ.  
4th Edition of the International Virtual Conference on Materials & Environmental Science, 18 - 27 November 2020, pp.15-21
- VII. **A NEW EQUATION TO CALCULATE THE CHEMICAL HARDNESS OF THE MOLECULES**  
KAYA S., SERDAROĞLU G., Katin K. P.  
5nd International Conference on Material Science and Technology, Kapadokya, Turkey, 16 October 2020, vol.5, pp.282
- VIII. **New Developments on the Application Maximum Entropy Principle: A Theoretical Study**  
SERDAROĞLU G., KAYA S.  
5nd International Conference on Material Science and Technology, Kapadokya, Turkey, 16 October 2020, vol.5, pp.281
- IX. **A triazolopyrimidine derivative as corrosion inhibitor for mild steel in HCl solution**  
Guo L., Yu R., Zhao J., Kaya S., Tan J., El Bakri Y.  
2nd International Symposium on Mechanics, Structures and Materials Science, MSMS 2020, Tianjin City, China, 28 - 29 March 2020, vol.2258
- X. **Quantum chemical calculations of chitosan as a green and efficient corrosion inhibitor on copper surface**  
BOURZI H., OUKHRIB R., HICHAM A., KAYA S., ISSAMI E., BAZZI L.  
International Conference on Green Chemistry and Sustainable Engineering, 23 - 25 July 2018
- XI. **Eser Analizde Sert ve Yumuşak Asit-Baz Yaklaşımının (HSAB) Önemi**  
KAYA S.  
International Trace Analysis Congress, Turkey, 20 - 23 June 2018
- XII. **Influence of the Alkyl Chain Length of Alkyltriazoles on the Corrosion Inhibition of Iron: A DFTB Study**  
Guo L., Wu M., KAYA S., Chen M., Madkoure L. H.  
International Symposium on Mechanics, Structures and Materials Science (MSMS), Tianjin, China, 9 - 10 June 2018, vol.1995
- XIII. **dft modeling and monte carlo simulation assessment of inhibition performance of some carbohydrazide schiff bases for stell corrosion**  
TÜZÜN B., KAYA S.

- international conference on technology, engineering and science, 26 - 29 October 2017
- XIV. **quantum chemical simulation studies on inhibition performances of some thiazole and thiadiazole derivatives against corrosion of iron**  
TÜZÜN B., KAYA S., KAYA C.  
2nd international gazi symposium series, 11 - 13 October 2017
- XV. **determination of corrosion inhibition effects of amino acids: quantum chemical and molecular dynamic simulation study**  
TÜZÜN B., KAYA S., KAYA C.  
2nd international gazi symposium series, 11 - 13 October 2017
- XVI. **investigation via principal component analysis dft and molecular dynamics simulations approaches on the anticorrosive effect of some thiophene derivatives against the corrosion of iron**  
TÜZÜN B., KAYA S.  
international congress on chemistry and materials science, 5 - 07 October 2017
- XVII. **theoretical evaluation of triazine derivatives as steel corrosion inhibitors monte carlo simulation approach**  
TÜZÜN B., KAYA S., KAYA C.  
3. international turkish congress on molecular spectroscopy, 26 - 29 August 2017
- XVIII. **Some New Applications in Solid State Chemistry of Chemical Hardness and Molar Volume Concepts**  
KAYA S., KAYA C.  
28. Ulusal Kimya Kongresi, Turkey, 15 - 21 August 2016
- XIX. **İyonik Kristallerin Örgü Enerjilerinin Hesaplanması İçin Yeni Bir Metot**  
KAYA S., KAYA C.  
5. ULUSAL ANORGANİK KİMYA KONGRESİ, Turkey, 22 - 25 April 2015
- XX. **İyonik Katılarda Örgü Enerjisi, Kohezif Enerji ve Mutlak Elektronegatiflik İlişkisinin İncelenmesi**  
KAYA S., KAYA C.  
5. ULUSAL ANORGANİK KİMYA KONGRESİ, Turkey, 22 - 25 April 2015
- XXI. **A new method for Calculation of Molecular Hardness**  
KAYA S., KAYA C.  
International Symposium on Molecular Chemistry, 19 December 2014
- XXII. **Kimyasal Sertliğin Kimyadaki Uygulamaları, Grup ve Moleküllerin Kimyasal Sertliğinin Hesaplanması için Yeni Bir Denklem**  
KAYA S., KAYA C.  
IV. Fiziksel Kimya Kongresi, Turkey, 5 - 08 June 2014
- XXIII. **Bazı iki dişli Schiff baz ligandlarının bakır(II) komplekslerinin hesaplamalı yöntemlerle yapısal analizi**  
ERKAN KARİPER S., KAYA S., KARAKAŞ D.  
IV Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013
- XXIV. **İzoelektronik Serilerde Kimyasal Sertlik, Katyonların İyonlaşma Enerjisi ve Elektron İlgilerinin Hesaplanması**  
KAYA S., KAYA C.  
IV. Ulusal Anorganik Kimya Kongresi, Turkey, 30 May - 02 June 2013

### **Activities in Scientific Journals**

TURKISH COMPUTATIONAL AND THEORETICAL CHEMISTRY, Committee Member, 2020 - Continues  
Arabian Journal of Chemical and Environmental Research, Committee Member, 2020 - Continues  
Journal of Applied Surfaces and Interfaces, Committee Member, 2020 - Continues  
Journal of Materials and Environmental Science, Committee Member, 2020 - Continues  
Far East Journal of Chemistry, Committee Member, 2020 - Continues

## Scientific Refereeing

JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, December 2021  
SURFACES AND INTERFACES, SCI Journal, December 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, December 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, December 2020  
Cumhuriyet Science Journal, National Scientific Refreed Journal, November 2020  
JOURNAL OF ALLOYS AND COMPOUNDS, SCI Journal, November 2020  
SURFACES AND INTERFACES, SCI Journal, November 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, October 2020  
TURKISH COMPUTATIONAL AND THEORETICAL CHEMISTRY, Other Indexed Journal, October 2020  
ERCİYES ÜNİVERSİTESİ FEN BİLİMLERİ ENSTİTÜSÜ DERGİSİ, National Scientific Refreed Journal, September 2020  
ARABIAN JOURNAL OF CHEMISTRY, SCI Journal, August 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, August 2020  
JOURNAL OF MOLECULAR STRUCTURE, Journal Indexed in SCI-E, July 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, July 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, July 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, June 2020  
Journal of Oleo Science , Other Indexed Journal, June 2020  
SUPERLATTICES AND MICROSTRUCTURES, SCI Journal, April 2020  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, National Scientific Refreed Journal, April 2020  
JOURNAL OF OLEO SCIENCE, National Scientific Refreed Journal, April 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, April 2020  
COMPUTATION, Other Indexed Journal, March 2020  
JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, March 2020  
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, SCI Journal, March 2020  
JOURNAL OF COMPUTATIONAL CHEMISTRY, SCI Journal, February 2020  
JOURNAL OF OLEO SCIENCE, Other Indexed Journal, February 2020  
CHEMICAL DATA COLLECTION, Other Indexed Journal, January 2020

## Scientific Research / Working Group Memberships

Kaya Research Group, Sivas Cumhuriyet University, Turkey, kayaresearchgroup.com, 2020 - Continues

## Metrics

Publication: 234  
Citation (WoS): 3165  
Citation (Scopus): 3417  
H-Index (WoS): 27  
H-Index (Scopus): 27

## Invited Talks

ANALYSIS OF THE RELATIONSHIP BETWEEN TOXICITY OF METAL CATIONS WITH QUANTUM CHEMICAL PARAMETERS,  
Conference, The Third Edition of The International Congress On Water And Environment Studies, Morocco, December  
2020