

## 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, 2017 - 2018, 2016 - 2017  
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, 2017 - 2018, 2016 - 2017  
Taşıma ve Depolama, Associate Degree, 2017 - 2018, 2016 - 2017  
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. **Phenolic compounds removal in table olive processing wastewater by column adsorption: conditions' optimization**  
Aziz K., Haydari I., KAYA S., Mandi L., Ouazzani N., Aziz F.  
Environmental Science and Pollution Research, vol.31, no.27, pp.38835-38845, 2024 (SCI-Expanded)
- II. **Low-cost materials as vehicles for pesticides in aquatic media: a review of the current status of different biosorbents employed, optimization by RSM approach**  
Aziz K., Mamouni R., KAYA S., Aziz F.  
Environmental Science and Pollution Research, vol.31, no.28, pp.39907-39944, 2024 (SCI-Expanded)
- III. **Spectroscopic, crystal structure and DFT-assisted studies of some nickel(II) chelates of a heterocyclic-based NNO donor aroylhydrazone: in vitro DNA binding and docking studies**  
Nair Y., Joy F., Vinod T., Vineetha M., Kurup M. R. P., KAYA S., SERDAROĞLU G., ERKAN S.  
Molecular Diversity, vol.28, no.2, pp.509-530, 2024 (SCI-Expanded)
- IV. **Chalcone-based novel mono and bistiocarbonylhydrazone: synthesis, crystal structure, antioxidant property and theoretical evaluation**  
Lafta A. Z., KAYA Y., ERÇAĞ A., Zorlu Y., KAYA S., Berisha A.  
Journal of Sulfur Chemistry, vol.45, no.3, pp.346-363, 2024 (SCI-Expanded)
- V. **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, vol.36, no.12, 2023 (SCI-Expanded)

- VI. **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, vol.36, no.12, 2023 (SCI-Expanded)
- VII. **Biological evaluation and in silico molecular docking studies of Abies cilicica (Antoine & Kotschy Carrière) resin**  
GÜÇLÜ G., TAŞ A., DİNÇER E., Ucar E., KAYA S., Berisha A., DURAL E., SİLİĞ Y.  
Journal of Molecular Structure, vol.1288, 2023 (SCI-Expanded)
- VIII. **Experimental and theoretical insights about the effect of some newly designed azomethine group-contained macroheterocycles on oxidative stress and DNA repair gene profiles in neuroblastoma cell lines**  
Cinar G., Agbektas T., Huseynzada A., Aliyeva G., Aghayev M., Hasanova U., KAYA S., Chtita S., Nour H., TAŞ A., et al.  
Journal of Molecular Structure, vol.1285, 2023 (SCI-Expanded)
- IX. **Synthesis and spectral investigation of novel 4-aryl-5-(aryldiazenyl)thiazole dyes festooned with fluorene moiety: Experimental and theoretical insight**  
El Guesmi N., Khormi A. Y., S Alzahrani A., Asghar B. H., KAYA S., Katin K. P., Farghaly T. A., Shaaban M. R., Farag A. M.  
Journal of Molecular Liquids, vol.383, 2023 (SCI-Expanded)
- X. **Effect of an imidazole-based ionic liquid as anti-corrosion additive on the performance of Al-air batteries**  
Guo L., Zhang Q., Huang Y., KAYA S., Zheng X., Zhang R., Shi W., Obot I. B.  
Journal of Electroanalytical Chemistry, vol.941, 2023 (SCI-Expanded)
- XI. **Analysis of boronic acids containing amino ferrocene by DFT approach and in silico studies**  
Muhammad U. S., ERKAN S., KAYA S.  
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- XII. **Iron-ligand complex, an efficient inhibitor of steel corrosion in hydrochloric acid media**  
Zaidi K., Bouroumane N., Merimi C., Aouinita A., Touzani R., Oussaid A., Hammouti B., Salim R., KAYA S., Ibrahim S. M.  
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- XIII. **Corrosion inhibition of mild steel in acidic media using new oxo-pyrimidine derivatives: Experimental and theoretical insights**  
Ferigita K. S. M., SARAÇOĞLU M., AlFalah M. G. K., YILMAZER M. İ., KÖKBUDAK Z., KAYA S., Kandemirli F.  
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- XIV. **DFT calculations of photophysical properties of ethylen-dioxy-thiophen derivatives oligomers with optoelectronic functionalities**  
Ninis O., El kharrim A., Agda F., Nebbach D., KAYA S., Abarkan M., Bouachrine M.  
Journal of Molecular Structure, vol.1284, 2023 (SCI-Expanded)
- XV. **Investigating the optical, electronic, magnetic properties and DFT of NiO films prepared using RF sputtering with various argon pressures**  
Hopoglu H., KAYA D., Maslov M. M., KAYA S., DEMİR İ., ALTUNTAŞ İ., UNGAN F., Akyol M., EKİCİBİL A., Tüzemen E.  
Physica B: Condensed Matter, vol.661, 2023 (SCI-Expanded)
- XVI. **Reactivity of diamanes against oxidation: A DFT study**  
KAYA S., Dua H., Sarkar U., Demin V. A., Kvashnin A. G.  
Chemical Physics, vol.571, 2023 (SCI-Expanded)
- XVII. **Changes in arginine metabolism in advanced Alzheimer's patients: Experimental and theoretical analyses**  
Sarı İ., Erşan S., Özmen E., Ayan D., Erşan E., Berisha A., KAYA S.  
Journal of Molecular Structure, vol.1282, 2023 (SCI-Expanded)
- XVIII. **Combination of doped amorphous carbon based dispersive solid phase extraction with ionic liquid-based DLLME for the extraction of aromatic amines from leather industries wastewater; Theoretical**

**and experimental insights**

Nemati M., Farajzadeh M. A., ALTUNAY N., Tuzen M., KAYA S., Maslov M. M., Afshar Mogaddam M. R.  
Journal of Molecular Structure, vol.1281, 2023 (SCI-Expanded)

- XIX. **Experimental and theoretical observations in a mixed mode dispersive solid phase extraction of exogenous surfactants from exhaled breath condensate prior to HPLC-MS/MS analysis**  
Khoubnasabjafari M., ALTUNAY N., Tuzen M., KAYA S., Katin K. P., Farajzadeh M. A., Hosseini M., Afshar Mogaddam M. R., Jouyban A.  
Journal of Molecular Structure, vol.1281, 2023 (SCI-Expanded)
- XX. **Effect of MgFe<sub>2</sub>O<sub>4</sub> catalyst preparation method on its surface characteristics and Fenton-like oxidation of tartrazine: Statistical comparison and DFT-assisted predation of mechanism**  
Soufi A., Khnifira M., Hajjaoui H., Abdennouri M., KAYA S., Bessbousse H., Barka N.  
Materials Today Communications, vol.35, 2023 (SCI-Expanded)
- XXI. **Adsorption of 40 low molecular weight drugs on pristine and fluorinated C<sub>60</sub> fullerenes: Ab initio, statistical and neural networks analysis**  
Kalika E. B., Bondarev N. V., Katin K. P., Kochaev A. I., Grekova A. A., KAYA S., Bauetdinov Y. A., Maslov M. M.  
Journal of Molecular Liquids, vol.377, 2023 (SCI-Expanded)
- XXII. **Acetylsalicylic acid as an environmentally friendly corrosion inhibitor for carbon steel XC48 in chloride environment**  
Merimi C., Hammouti B., Zaidi K., Hafez B., Elmsellem H., Touzani R., KAYA S.  
Journal of Molecular Structure, vol.1278, 2023 (SCI-Expanded)
- XXIII. **Copper(II) chelates derived from an N,N,O-tridentate 2-pyridinecarboxaldehyde-N4-phenylsemicarbazone: Synthesis, spectral aspects, crystal structure, FMO and NBO analysis**  
Sithambaresan M., Kurup M. R. P., SERDAROĞLU G., KAYA S.  
Journal of Molecular Structure, vol.1277, 2023 (SCI-Expanded)
- XXIV. **Experimental and density functional theoretical analyses on degradation of acid orange 7 via UV irradiation and ultrasound enhanced by fenton process**  
YILDIZ S., Canbaz G., KAYA S., Maslov M. M.  
Journal of Molecular Structure, vol.1277, 2023 (SCI-Expanded)
- XXV. **Unraveling Bonding Mechanisms and Electronic Structure of Pyridine Oximes on Fe(110) Surface: Deeper Insights from DFT, Molecular Dynamics and SCC-DFT Tight Binding Simulations**  
Lgaz H., Lee H., KAYA S., Salghi R., Ibrahim S. M., Chafiq M., Bazzi L., Ko Y. G.  
Molecules, vol.28, no.8, 2023 (SCI-Expanded)
- XXVI. **Equilibrium and DFT modeling studies for the biosorption of Safranin O dye from water samples using Bacillus subtilis biosorbent**  
ÇETİNKAYA S., KAYA S., Aksu A., ÇETİNTAŞ H. İ., Jalbani N. S., ERKAN S., Marzouki R.  
Journal of Molecular Structure, vol.1276, 2023 (SCI-Expanded)
- XXVII. **Prunus mahaleb shell as a sustainable bioresource for carminic acid removal from aqueous solution: Experimental and theoretical studies**  
Keskin Z. S., Şenol Z. M., Kaya S., Şimşek S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1275, pp.1-11, 2023 (SCI-Expanded)
- XXVIII. **Adsorption mechanism investigation of methylthioninium chloride dye onto some metal phosphates using Monte Carlo dynamic simulations and DFT calculations**  
Attarki J., Khnifira M., Boumya W., Mahsoun A., Lemdek E., Sadiq M., Abdennouri M., KAYA S., Barka N.  
Inorganic Chemistry Communications, vol.149, 2023 (SCI-Expanded)
- XXIX. **A detailed electronic-scale DFT modeling/MD simulation, electrochemical and surface morphological explorations of imidazolium-based ionic liquids as sustainable and non-toxic corrosion inhibitors for mild steel in 1 M HCl**  
EL Hajjaji F., Ech-chihbi E., Salim R., Titi A., Messali M., El Ibrahim B., KAYA S., Taleb M.  
Materials Science and Engineering B: Solid-State Materials for Advanced Technology, vol.289, 2023 (SCI-Expanded)
- XXX. **Experimental and theoretical insights about the effect of some newly designed azomethine group-**

**contained macroheterocycles on oxidative stress and DNA repair gene profiles in neuroblastoma cell lines**

Çınar G., Ağbektas T., Huseynzada A., Aliyeva G., Aghayev M., Hasanova U., Kaya S., Chtita S., Nour H., Taş A., et al.  
JOURNAL OF MOLECULAR STRUCTURE, pp.2-16, 2023 (SCI-Expanded)

- XXXI. **Green synthesis of reduced graphene oxide and their use on column adsorption of phenol from olive mill wastewater**  
Haydari I., Aziz K., Kaya S., Daştan T., Ouazzani N., Mandi L., Aziz F.  
Process Safety and Environmental Protection, vol.170, pp.1079-1091, 2023 (SCI-Expanded)
- XXXII. **Experimental and theoretical insights on the structural and optical properties of GeOx thin films deposited via RF magnetron sputtering under varying oxygen percentage**  
ŞENADIM TÜZEMEN E., Hopoğlu H., SARITAŞ S., AYDINOĞLU H. S., ERTUĞRUL M., Maslov M., KAYA S., UNGAN F., GÜR E.  
Physica B: Condensed Matter, vol.650, 2023 (SCI-Expanded)
- XXXIII. **Adsorption properties of amine modified lignin-hydrogel composite for uranyl ions: Theoretical and experimental insights**  
ŞİMŞEK S., KAYA S., Jalbani N. S.  
Journal of the Indian Chemical Society, vol.100, no.2, 2023 (SCI-Expanded)
- XXXIV. **Anisotropic Carrier Mobility and Spectral Fingerprints of Two-Dimensional  $\gamma$ -Phosphorus Carbide with Antisite Defects**  
Katin K. P., Maslov M. M., Nikitenko V. R., Kochoev A. I., KAYA S., Prezhdo O. V.  
Journal of Physical Chemistry Letters, vol.14, no.1, pp.214-220, 2023 (SCI-Expanded)
- XXXV. **Synthesis and spectral properties of novel series of fluorene-based azo dyes containing thiazole scaffold: Studying of the solvent and substituent effect on absorption spectra**  
ElGuesmi N., Farghaly T., Khormi A. Y., Shaaban M. R., Katin K. P., KAYA S.  
Journal of Molecular Structure, vol.1271, 2023 (SCI-Expanded)
- XXXVI. **An effective and smart corrosion inhibitor in acidic environment: Experimental & theoretical studies**  
Bouoidina A., Haldhar R., Salim R., Ech-chihbi E., Ichou H., El-Hajjaji F., Kim S., El Ibrahim B., KAYA S., Taleb M.  
Korean Journal of Chemical Engineering, vol.40, no.1, pp.235-247, 2023 (SCI-Expanded)
- XXXVII. **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, vol.37, no.10, pp.1649-1665, 2023 (SCI-Expanded)
- XXXVIII. **Recent Trends in the Characterization and Application Progress of Nano-Modified Coatings in Corrosion Mitigation of Metals and Alloys**  
Thakur A., KAYA S., Kumar A.  
Applied Sciences (Switzerland), vol.13, no.2, 2023 (SCI-Expanded)
- XXXIX. **Metal cations toxicity: An inorganic interpretation**  
KAYA S., Bezerra C. W., Fernandes de Farias R., Çiltaş A., ELİK M.  
Journal of the Indian Chemical Society, vol.100, no.1, 2023 (SCI-Expanded)
- XL. **Biosorption of lead ions (Pb<sup>2+</sup>) from water samples using dried Lemna minor biomass: experimental and density functional theory studies**  
KAYA S., ÇETİNKAYA S., Jalbani N. S., YENİDÜNYA A. F., KÜTÜK N., KASAKA E., Maslov M. M.  
Biomass Conversion and Biorefinery, 2023 (SCI-Expanded)
- XLI. **Advancement of corrosion inhibitor system through N-heterocyclic compounds: a review**  
Sheetal S., Batra R., Singh A. K., Singh M., Thakur S., Pani B., KAYA S.  
Corrosion Engineering Science and Technology, vol.58, no.1, pp.73-101, 2023 (SCI-Expanded)
- XLII. **A Combined Study on Degradation Mechanism of Reactive Orange 16 through Fenton-like Process: Experimental Studies and Density Functional Theoretical Findings**  
YILDIZ S., TOPAL CANBAZ G., KAYA S., Maslov M. M.  
ChemistrySelect, vol.7, no.48, 2022 (SCI-Expanded)
- XLIII. **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 (SCI-Expanded)

- XLIV. **Synthesis of new halogenated compounds based on 8-hydroxyquinoline derivatives for the inhibition of acid corrosion: Theoretical and experimental investigations**  
Rbaa M., Galai M., Ouakki M., Hsissou R., Berisha A., KAYA S., Berdimurodov E., Lakhrissi B., Zarrouk A.  
MATERIALS TODAY COMMUNICATIONS, vol.33, 2022 (SCI-Expanded)
- XLV. **Elucidating the adsorption mechanisms of anionic dyes on chitosan (110) surface in aqueous medium by quantum chemical and molecular dynamics**  
Khnifira M., Boumya W., Attarki J., Mahsoun A., Abdennouri M., Sadiq M. ', KAYA S., Barka N.  
MATERIALS TODAY COMMUNICATIONS, vol.33, 2022 (SCI-Expanded)
- XLVI. **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 (SCI-Expanded)
- XLVII. **Multilayer perceptron neural network-based QSAR models for the assessment and prediction of corrosion inhibition performances of ionic liquids**  
Quadri T. W., Olasunkanmi L. O., Fayemi O. E., Akpan E. D., Lee H. S., Lgaz H., Verma C., Guo L., KAYA S., Ebenso E. E.  
COMPUTATIONAL MATERIALS SCIENCE, vol.214, 2022 (SCI-Expanded)
- XLVIII. **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 (SCI-Expanded)
- XLIX. **Recent Advancements in Surface Modification, Characterization and Functionalization for Enhancing the Biocompatibility and Corrosion Resistance of Biomedical Implants**  
Thakur A., Kumar A., KAYA S., Marzouki R., Zhang F., Guo L.  
COATINGS, vol.12, no.10, 2022 (SCI-Expanded)
- L. **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 (SCI-Expanded)
- LI. **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 (SCI-Expanded)
- LII. **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 (SCI-Expanded)
- LIII. **Enhancement corrosion resistance of mild steel in 15% HCl solution by a novel bio-based polyurethane for oil well acidizing**  
Rahimi A., Abdouss M., Farhadian A., Guo L., KAYA S., Neshati J.  
JOURNAL OF INDUSTRIAL AND ENGINEERING CHEMISTRY, vol.113, pp.332-347, 2022 (SCI-Expanded)
- LIV. **Theoretical investigations on the unimolecular decomposition mechanisms of isopropyl acetate**  
Abdel-Rahman M. A., Shiroudi A., KAYA S., El-Nahas A. M.  
Journal of Molecular Structure, vol.1262, 2022 (SCI-Expanded)
- LV. **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 (SCI-Expanded)
- LVI. **High-Performance Material for the Effective Removal of Uranyl Ion from Solution: Computationally**

### Supported Experimental Studies

Şimşek S., Derin Y., Kaya S., Hasdemir Z. M., Katin K. P., Özer A.  
LANGMUIR, vol.1, no.1, pp.1-16, 2022 (SCI-Expanded)

- LVII. **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**  
Hssissou 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 (SCI-Expanded)
- LVIII. **Inhibitive performance of novel/eco-friendly pyrimidine derivative for Q235 steel protection in 15% HCl under hydrodynamic condition: Combination of experimental, surface and computational approach**  
Singh A., Ansari K. R., Lin Y., Ali I. H., KAYA S., El Ibrahim B.  
MATERIALS TODAY COMMUNICATIONS, vol.32, 2022 (SCI-Expanded)
- LIX. **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 (SCI-Expanded)
- LX. **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, vol.126, no.27, pp.4507-4516, 2022 (SCI-Expanded)
- LXI. **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, vol.36, no.7, 2022 (SCI-Expanded)
- LXII. **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 R.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1259, 2022 (SCI-Expanded)
- LXIII. **Experimental and density functional theoretical modeling of triazole pesticides extraction by Ti<sub>2</sub>C 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., Nemat M.  
Microchemical Journal, vol.178, 2022 (SCI-Expanded)
- LXIV. **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 (SCI-Expanded)
- LXV. **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 (SCI-Expanded)
- LXVI. **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., Nemat M., ALTUNAY N., Tuzen M., KAYA S., Kheradmand F., Afshar Mogaddam M. R.  
Microchemical Journal, vol.177, 2022 (SCI-Expanded)
- LXVII. **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, vol.76, no.6, pp.3413-3423, 2022 (SCI-Expanded)
- LXVIII. **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.

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- CXXXI. **Chemically modified guar gum and ethyl acrylate composite as a new corrosion inhibitor for reduction in hydrogen evolution and tubular steel corrosion protection in acidic environment**  
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- CXXXII. **Band dispersion and optical gain calculations of staggered type**

**GaAs<sub>0.4</sub>Sb<sub>0.6</sub>/In<sub>0.7</sub>Ga<sub>0.3</sub>As/GaAs<sub>0.4</sub>Sb<sub>0.6</sub> nano-heterostructure under electric field and [100] strain**

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- XVIII. **Lattice Energies from Hydration Enthalpies: Some acid-base and Structural Considerations**  
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- XIX. **Corrosion inhibition studies for mild steel in 5.0 M HCl by substituted phenyltetrazole**  
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- XX. **Conceptual Density Functional Theoretical Investigation of the Corrosion Inhibition Efficiencies of Some Molecules Containing Mercapto (-SH) Group**  
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- XXI. **Effect of Molecular Hardness on Ionic Characters, Bond Lengths, Bond Force Constants and Melting Points of Alkali Halides**  
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- XXII. **Theoretical Investigation of Corrosion Inhibition of Iron Metal by Some Benzothiazole Derivatives: A Monte Carlo Study**  
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- XXIII. **Validation of the Charge Equalization Principles during the Formation of Small Molecules**  
KAYA S., KAYA C., ISLAM N., OBOT I. B.  
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- XXIV. **Comments on Electronegativity Equalization with Pauling Units**  
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- XXV. **A Useful Method for the Prediction of Molecular Electrophilicity and Nucleophilicity**  
KAYA S., KAYA C., UĞURLU İ., ISLAM N.  
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.3, no.2, pp.89-102, 2016 (Peer-Reviewed Journal)
- XXVI. **Derivation of ionization energy and electron affinity equations using chemical hardness and absolute electronegativity in isoelectronic series**  
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- XXVII. **Investigation of relationship with electron configuration of chemical hardness, absolute**

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Journal of Physical and Theoretical Chemistry, pp.1-13, 2014 (Peer-Reviewed Journal)

XXVIII. **EFFECT OF SOME ELECTRON DONOR AND ELECTRON ACCEPTOR GROUPS ON STABILITY OF COMPLEXES ACCORDING TO THE PRINCIPLE OF HSAB**

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## **Books & Book Chapters**

I. **Materials Development and Processing for Biomedical Applications**

KAYA S., Yesudass S., Arthanari S., Bose S., SERDAROĞLU G.

CRC PRESS/ Taylor & Francis Group, Florida, 2022

II. **Organic and Inorganic Corrosion Inhibitors A Comparison**

SERDAROĞLU G., KAYA S.

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III. **Computational methods used in corrosion inhibition research**

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in: Eco-Friendly Corrosion Inhibitors Principles, Designing and Applications, Guo Lei, Verma, Chandrabhan, Zhang, Dawei, Editor, Elsevier, Amsterdam, pp.527-538, 2022

IV. **Ionic Liquids as Corrosion Inhibitors**

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V. **New Challenges and Industrial Applications for Corrosion Prevention and Control**

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VI. **Phthalonitrile Derivatives Containing Different Heterocyclic Groups as New Corrosion Inhibitors for Iron(110) Surface**

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VII. **CONCEPTUAL DENSITY FUNCTIONAL THEORY AND ITS APPLICATIONS IN THE CHEMICAL DOMAIN**

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VIII. **Conceptual Density Functional Theory and Its Application to Corrosion Inhibition Studies**

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IX. **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

X. **Ionization Energies of Atoms of 103 Elements of Periodic Table Using Semiempirical and DFT Methods**

ISLAM N., KAYA S., GHOSH D. C.

## Refereed Congress / Symposium Publications in Proceedings

- I. **EFFECT OF HETEROCYCLIC COMPOUNDS CONTAINING AZOMETHINE GROUP ON OXIDATIVE STRESS AND DNA REPAIR GENE PROFILES IN NEUROBLASTOMA CELL LINES: In Silico and In Vitro ANALYSIS**  
CINAR G., AĞBEKTAŞ T., Huseynzada A., Gunel A., Mirjavid A., Hasanova U., Chtita S., KAYA S., TAŞ A., SİLİĞ Y.  
Internatiol Conference on Physical Chemistry/Functional Materials (PCMF22), Turkey, 23 June 2022
- II. **THE EFFECT OF AZOMETINE GROUP COMPOUNDS CONTAINING SCHIFF BASE ON EXPRESSION PROFILES OF GENES INVOLVED IN WNT AND MAPK PATHWAY IN LUNG CANCER CELL LINES: In Silico and In Vitro ANALYSIS**  
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Internatiol Conference on Physical Chemistry/Functional Materials (PCMF22), Turkey, 23 June 2022
- III. **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
- IV. **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
- V. **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
- 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. **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
- VIII. **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
- IX. **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
- X. **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

- XI. **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
- XII. **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
- XIII. **Eser Analizde Sert ve Yumuşak Asit-Baz Yaklaşımının (HSAB) Önemi**  
KAYA S.  
International Trace Analysis Congress, Turkey, 20 - 23 June 2018
- XIV. **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
- XV. **dft modeling and monte carlo simulation assessment of inhibition performance of some carbonyl Schiff bases for steel corrosion**  
TÜZÜN B., KAYA S.  
international conference on technology, engineering and science, 26 - 29 October 2017
- XVI. **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
- XVII. **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
- XVIII. **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
- XIX. **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
- XX. **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
- XXI. **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
- XXII. **İyonik Kristallerin Örgü Enerjilerinin Hesaplanması İçin Yeni Bir Metot**  
KAYA S., KAYA C.  
5. ULUSAL ANORGANİK KİMYA KONGRESİ, Turkey, 22 - 25 April 2015
- XXIII. **A new method for Calculation of Molecular Hardness**  
KAYA S., KAYA C.  
International Symposium on Molecular Chemistry, 19 December 2014
- XXIV. **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

XXV. **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

XXVI. **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

JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, December 2020

SURFACES AND INTERFACES, 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

JOURNAL OF MOLECULAR LIQUIDS, SCI Journal, August 2020

ARABIAN JOURNAL OF CHEMISTRY, 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

COMPUTATIONAL AND THEORETICAL CHEMISTRY, National Scientific Refreed Journal, April 2020

SUPERLATTICES AND MICROSTRUCTURES, SCI 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, Türkiye, kayaresearchgroup.com, 2020 - Continues

### **Metrics**

Publication: 294

Citation (WoS): 3502

Citation (Scopus): 6326

H-Index (WoS): 29

H-Index (Scopus): 43

### **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