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Kişisel Bilgiler

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Eğitim Bilgileri

Doktora, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2013 - 2017

Yüksek Lisans, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2011 - 2013

Lisans, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, Türkiye 2007 - 2011

Yaptığı Tezler

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

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

Araştırma Alanları

Kimya

Akademik Unvanlar / Görevler

Doç.Dr., Sivas Cumhuriyet Üniversitesi, Sağlık Hizmetleri Meslek Yüksekokulu, Eczacılık Bölümü, 2013 - Devam Ediyor

Akademik İdari Deneyim

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

Verdiği Dersler

Temel Kimya, Ön Lisans, 2020 - 2021

Çevre Sağlığı ve Koruma, Ön Lisans, 2020 - 2021

Temel Kimya, Ön Lisans, 2020 - 2021

İtfaiye Araç ve Malzeme Bilgisi - II, Ön Lisans, 2018 - 2019

Yapı ve Elektrik İşlerinde İSG, Ön Lisans, 2018 - 2019

Arama Kurtarma Teknikleri, Ön Lisans, 2018 - 2019

İş Sağlığı ve Güvenliği Risk Analizi, Ön Lisans, 2019 - 2020

Genel Kimya, Ön Lisans, 2019 - 2020

İş Kazaları ve Raporlama, Ön Lisans, 2018 - 2019

Toksikoloji ve Zehirlenmeler, Ön Lisans, 2019 - 2020
Temel Elektrik ve Elektronik Bilgisi, Ön Lisans, 2018 - 2019
Kımyasallar ve Tehlikeleri, Ön Lisans, 2018 - 2019
İtfaiye Araç ve Malzeme Bilgisi - I, Ön Lisans, 2018 - 2019
Toksikoloji ve Zehirlenmeler, Ön Lisans, 2017 - 2018, 2016 - 2017
Taşıma ve Depolama, Ön Lisans, 2017 - 2018
Uyarı İşaretleri ve Levha Standartları, Ön Lisans, 2018 - 2019
Kımyasallar ve Tehlikeleri, Ön Lisans, 2017 - 2018
Genel Kimya, Ön Lisans, 2017 - 2018, 2016 - 2017
Taşıma ve Depolama, Ön Lisans, 2017 - 2018, 2016 - 2017
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Matematik 2, Ön Lisans, 2016 - 2017
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İngilizce - I, Ön Lisans, 2016 - 2017
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Atatürk İlkeleri ve İnkılap Tarihi - I, Ön Lisans, 2014 - 2015
Ticari Matematik, Ön Lisans, 2013 - 2014
Bilgisayarlı Muhasebe, Ön Lisans, 2013 - 2014

Jüri Üyelikleri

Yarışma, TÜBİTAK - 2204 - B ORTAOKUL ÖĞRENCİLERİ ARAŞTIRMA PROJELERİ YARIŞMASI, TÜBİTAK, Ekim, 2020

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- I. 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.
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- II. Can van der Waals constants be used in the chemical reactivity analysis? A new approach as a support to minimum magnetizability principle
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- IV. 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
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- V. Synthesis and spectral investigation of novel 4-aryl-5-(aryldiazenyl)thiazole dyes festooned with fluorene moiety: Experimental and theoretical insight
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- M.
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- VI. **Effect of an imidazole-based ionic liquid as anti-corrosion additive on the performance of Al-air batteries**
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- VII. **Iron-ligand complex, an efficient inhibitor of steel corrosion in hydrochloric acid media**
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- VIII. **Investigating the optical, electronic, magnetic properties and DFT of NiO films prepared using RF sputtering with various argon pressures**
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- IX. **Corrosion inhibition of mild steel in acidic media using new oxo-pyrimidine derivatives: Experimental and theoretical insights**
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- X. **Analysis of boronic acids containing amino ferrocene by DFT approach and in silico studies**
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- XI. **DFT calculations of photophysical properties of ethylen-dioxy-thiophen derivatives oligomers with optoelectronic functionalities**
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- XII. **Reactivity of diamanes against oxidation: A DFT study**
KAYA S., Dua H., Sarkar U., Demin V. A., Kvashnin A. G.
Chemical Physics, cilt.571, 2023 (SCI-Expanded)
- XIII. **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.
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- XIV. **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.
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- XV. **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.
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- XVI. **Effect of MgFe2O4 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.
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- XVII. **Adsorption of 40 low molecular weight drugs on pristine and fluorinated C60 fullerenes: Ab initio, statistical and neural networks analysis**
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- XVIII. **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.
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- XIX. **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.
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- XX. **Experimental and density functional theoretical analyses on degradation of acid orange 7 via UV irradiation and ultrasound enhanced by fenton process**
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- XXI. **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**
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- XXII. **Equilibrium and DFT modeling studies for the biosorption of Safranin O dye from water samples using Bacillus subtilis biosorbent**
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- XXIII. **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.
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- XXIV. **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**
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- XXV. **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 Ibrahimi B., KAYA S., Taleb M.
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- XXVI. **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., Mahsouna A., Lemdek E., Sadiq M., Abdennouri M., KAYA S., Barka N.
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- XXVII. **Adsorption properties of amine modified lignin-hydrogel composite for uranyl ions: Theoretical and experimental insights**
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- XXVIII. **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.
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- XXIX. **Green synthesis of reduced graphene oxide and their use on column adsorption of phenol from olive mill wastewater**
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- XXX. **Anisotropic Carrier Mobility and Spectral Fingerprints of Two-Dimensional γ-Phosphorus Carbide with Antisite Defects**

- Katin K. P., Maslov M. M., Nikitenko V. R., Kochaev A. I., KAYA S., Prezhdo O. V.
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- XXXI. **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**
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- XXXII. **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.
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- XXXIII. **Low-cost materials as vehicles for pesticides in aquatic media: a review of the current status of different biosorbents employed, optimization by RSM approach**
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- XXXIV. **Spectroscopic, crystal structure and DFT-assisted studies of some nickel(II) chelates of a heterocyclic-based NNO donor arylhydrazone: in vitro DNA binding and docking studies**
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- XXXV. **Advancement of corrosion inhibitor system through N-heterocyclic compounds: a review**
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- XXXVI. **An effective and smart corrosion inhibitor in acidic environment: Experimental & theoretical studies**
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- XXXVII. **Phenolic compounds removal in table olive processing wastewater by column adsorption: conditions' optimization**
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- XXXVIII. **Biosorption of lead ions (Pb^{2+}) 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.
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- XXXIX. **Metal cations toxicity: An inorganic interpretation**
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- XL. **Quantum chemical and molecular dynamics simulation approach to investigate adsorption behaviour of organic azo dyes on TiO_2 and ZnO surfaces**
Mandal S., Zamindar S., Sarkar S., Murmu M., Guo L., KAYA S., Hirani H., Banerjee P.
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- XLI. **A Combined Study on Degradation Mechanism of Reactive Orange 16 through Fenton-like Process: Experimental Studies and Density Functional Theoretical Findings**
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- XLII. **Molecular dynamic simulations and computational DFT of adsorption performances of malachite green on the metal fluorides in aqueous medium**
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- XLIII. **Elucidating the adsorption mechanisms of anionic dyes on chitosan (110) surface in aqueous medium by quantum chemical and molecular dynamics**
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- XLIV. Synthesis of new halogenated compounds based on 8-hydroxyquinoline derivatives for the inhibition of acid corrosion: Theoretical and experimental investigations**
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- XLV. Multilayer perceptron neural network-based QSAR models for the assessment and prediction of corrosion inhibition performances of ionic liquids**
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- XLVI. Effect of electron donors on the photophysical and theoretical properties of BODIPY dyes based on tetrazolo[1,5-a]quinoline**
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- XLVII. Recent Advancements in Surface Modification, Characterization and Functionalization for Enhancing the Biocompatibility and Corrosion Resistance of Biomedical Implants**
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 COATINGS, cilt.12, sa.10, 2022 (SCI-Expanded)
- XLVIII. Adsorption study of N (-benzo[d]thiazol-2-yl)-1-(thiophene-2-yl) methanimine at mild steel/aqueous H₂SO₄ interface**
 Singh A. K., Singh M., Thakur S., Pani B., KAYA S., EL Ibrahim B., Marzouki R.
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- XLIX. 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.
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- L. 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**
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- LI. 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.
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- LII. 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.
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- LIII. Theoretical investigations on the unimolecular decomposition mechanisms of isopropyl acetate**
 Abdel-Rahman M. A., Shiroudi A., KAYA S., El-Nahas A. M.
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- LIV. 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**
 Hsisou R., Azogagh M., Benhiba F., Echihi S., Galai M., Shaim A., Bahaj H., Briche S., KAYA S., Serdaroglu G., et al.
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- LV. Effect of Hemp Fiber Addition on Mechanical Properties of Acrylic Resin: Coupled Experimental and Theoretical Study**
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- LVI. 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.

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- LVII. 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.
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- LVIII. 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.
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- LIX. On the Prediction of Lattice Energy with the Fukui Potential: Some Supports on Hardness Maximization in Inorganic Solids
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- LX. Handling Keywords: MXene Nanomaterial Hazardous pollutant Adsorption Environmental remediation
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- LXI. Crystal chemistry, DFT calculation and optical properties of the double perovskite stannate Sr₂Sn_{0.8}In_{0.8}W_{0.4}O₆
Belgacem B., Maslov M. M., KAYA S., Ali I. H., Ben Hassen R.
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- LXII. 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.
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- LXIII. New mixed-ligand iron(III) complexes containing thiocarbohydrazones: Preparation, characterization, and chemical reactivity analysis through theoretical calculations
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- LXIV. 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.
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- LXV. Mathematical modeling studies for the adsorptive removal of ciprofloxacin drug from water samples using functionalized silica resin
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- LXVI. Experimental and density functional theory studies during a new solid phase extraction of phenolic compounds from wastewater samples prior to GC-MS determination
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- LXVII. Fluorinated carbon and boron nitride fullerenes for drug Delivery: Computational study of structure and adsorption
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- LXVIII. 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.
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- LXIX. An insight about the interaction of Aryl Benzothiazoles with mild steel surface in aqueous HCl solution

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- LXX. **Theoretical and experimental insights about the adsorption of uranyl ion on a new designed Vermiculite-Polymer composite**
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- LXXI. **Natural corrosion inhibitor of renewable eco-waste for SS-410 in sulfuric acid medium: adsorption, electrochemical, and computational studies**
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- LXXIII. **One-Pot Hydrothermal Synthesized Nitrogen and Sulfur Codoped Carbon Dots for Acid Corrosion Inhibition of Q235 Steel br**
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- LXXXIII. **An experimental and theoretical approach to electrochemical sensing of environmentally hazardous dihydroxy benzene isomers at polysorbate modified carbon paste electrode**

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- LXXXV. **Experimental and DFT Modeling Studies for the Adsorptive Removal of Reactive Dyes from Wastewater**

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- LXXXVI. **Non-fullerene acceptor IDIC based on indacinodithiophene used as an electron donor for organic solar cells: A computational study**

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- LXXXVII. **DFT computational study of trihalogenated aniline derivative's adsorption onto graphene/fullerene/fullerene-like nanocages, X₁₂Y₁₂ (X = Al, B, and Y = N, P)**

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- LXXXVIII. **A benzimidazolium salt as effective corrosion inhibitor against the corrosion of mild steel in acidic medium: experimental and theoretical studies**

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- LXXXIX. **Recent Innovations in Nano Container-Based Self-Healing Coatings in the Construction Industry**

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- XC. **Detailed Electronic Structure, Physico-Chemical Properties, Excited State Properties, Virtual Bioactivity Screening and SERS Analysis of Three Guanine Based Antiviral Drugs Valacyclovir HCl Hydrate, Acyclovir and Ganciclovir**

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- XCI. **Conformational Analysis, Spectroscopic Insights, Chemical Descriptors, ELF, LOL and Molecular Docking Studies of Potential Pyrimidine Derivative with Biological Activities**

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- XCII. **Equilibrium, thermodynamic, and kinetic modeling studies for the adsorptive removal of oxyanions from water**

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- XCIII. **Sour corrosion of C1018 carbon steel and its inhibition by 1-benzylimidazole: electrochemical, SEM, FTIR and computational assessment**

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- XCIV. **Spectral studies and quantum chemical ab initio calculations for Copper(II) complexes of two heterocyclic arylhydrazones**

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- XCVI. **Performance of curing epoxy resin as potential anticorrosive coating for carbon steel in 3.5% NaCl medium: Combining experimental and computational approaches**
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- XCVII. **Novel bromide-cucurbit[7]uril supramolecular ionic liquid as a green corrosion inhibitor for the oil and gas industry**
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- XCIX. **Inhibition effect of newly synthesized benzoxanthonesderivative on hydrogen evolution and Q235 steelcorrosion in 15% HCl under hydrodynamic condition: Combination of experimental, surface and computational study**
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- CII. **Application of pyrrolidinomethylcalix[4]arene coated silica adsorbent for the removal of Chicago sky blue 6B dye from water samples: Equilibrium and computational modelling studies**
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- CXI. **Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries**
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- CXV. **Two empirical formulae for estimating standard entropy of inorganic ionic solids and a possible connection between two associated electronic structure principles**
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- CXVII. **New imidazolium ionic liquids as ecofriendly corrosion inhibitors for mild steel in hydrochloric acid (1 M): Experimental and theoretical approach**
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- CXX. **Investigations of Hg(II) analysis in real samples via computational chemistry, experimental design, and green microextraction approach**
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Metrikler

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Davetli Konuşmalar

ANALYSIS OF THE RELATIONSHIP BETWEEN TOXICITY OF METAL CATIONS WITH QUANTUM CHEMICAL PARAMETERS,

