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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
Kimyasallar 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
Kimyasallar ve Tehlikeleri, Ön Lisans, 2017 - 2018
Genel Kimya, Ön Lisans, 2017 - 2018, 2016 - 2017
Taşıma ve Depolama, Ön Lisans, 2017 - 2018, 2016 - 2017
Matematik - I, Ön Lisans, 2016 - 2017
Matematik 2, Ön Lisans, 2016 - 2017
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İngilizce - I, Ön Lisans, 2016 - 2017
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Bilgisayar - 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. **Phenolic compounds removal in table olive processing wastewater by column adsorption: conditions' optimization**
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Environmental Science and Pollution Research, cilt.31, sa.27, ss.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**
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- 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**
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- IV. **Chalcone-based novel mono and bistiocarbonylhydrazone: synthesis, crystal structure, antioxidant property and theoretical evaluation**
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- V. **Removal of erythrosine B dye from wastewater using chitosan boric acid composite material: Experimental and density functional theory findings**
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- VI. **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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- VII. **Biological evaluation and in silico molecular docking studies of Abies cilicica (Antoine & Kotschy Carrière) resin**
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- 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.
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- 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.
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- 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.
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- XI. **Analysis of boronic acids containing amino ferrocene by DFT approach and in silico studies**
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- 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.
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- 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.
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- 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.
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- 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.
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- XVI. **Reactivity of diamanes against oxidation: A DFT study**
KAYA S., Dua H., Sarkar U., Demin V. A., Kvashnin A. G.
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- 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.
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- 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, cilt.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.
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- XX. 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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- XXI. Adsorption of 40 low molecular weight drugs on pristine and fluorinated C₆₀ 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.
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- 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.
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- 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.
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- 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.
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- 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.
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- XXVI. Equilibrium and DFT modeling studies for the biosorption of Safranin O dye from water samples using Bacillus subtilis biosorbent**
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- 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.
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- 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.
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- 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.
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- 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., Ağbektaş T., Huseynzada A., Aliyeva G., Aghayev M., Hasanova U., Kaya S., Chtita S., Nour H., Taş A., et al.

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- 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.
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- XXXII. **Experimental and theoretical insights on the structural and optical properties of GeO_x 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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- XXXIII. **Adsorption properties of amine modified lignin-hydrogel composite for uranyl ions: Theoretical and experimental insights**
ŞİMŞEK S., KAYA S., Jalbani N. S.
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- XXXIV. **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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- 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.
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- XXXVI. **An effective and smart corrosion inhibitor in acidic environment: Experimental & theoretical studies**
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- XXXVII. **Quantum chemical and molecular dynamics simulation approach to investigate adsorption behaviour of organic azo dyes on TiO₂ and ZnO surfaces**
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- 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.
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- XXXIX. **Metal cations toxicity: An inorganic interpretation**
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- XL. **Biosorption of lead ions (Pb²⁺) from water samples using dried Lemna minor biomass: experimental and density functional theory studies**
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- 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.
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- XLII. **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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- XLIII. **Molecular dynamic simulations and computational DFT of adsorption performances of malachite green on the metal fluorides in aqueous medium**
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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. **Elucidating the adsorption mechanisms of anionic dyes on chitosan (110) surface in aqueous medium by quantum chemical and molecular dynamics**
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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. **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, cilt.214, 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. **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.
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- 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.
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- 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**
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- 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.
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- 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.
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- LIV. **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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- 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.
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- LVI. **High-Performance Material for the Effective Removal of Uranyl Ion from Solution: Computationally Supported Experimental Studies**
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- 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**
Hsissou 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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- 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.
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- 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.
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- LX. **On the Prediction of Lattice Energy with the Fukui Potential: Some Supports on Hardness Maximization in Inorganic Solids**
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- 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.
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- LXII. **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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- LXIII. **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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- 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.
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- 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.
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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. **Mathematical modeling studies for the adsorptive removal of ciprofloxacin drug from water samples using functionalized silica resin**
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- LXVIII. **An insight about the interaction of Aryl Benzothiazoles with mild steel surface in aqueous HCl solution**
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- LXIX. **Computational and experimental studies on the corrosion inhibition performance of an aerial extract of Cnicus Benedictus weed on the acidic corrosion of mild steel**

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- LXX. **Fluorinated carbon and boron nitride fullerenes for drug Delivery: Computational study of structure and adsorption**
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- LXXI. **Theoretical and experimental insights about the adsorption of uranyl ion on a new designed Vermiculite-Polymer composite**
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- LXXII. **Natural corrosion inhibitor of renewable eco-waste for SS-410 in sulfuric acid medium: adsorption, electrochemical, and computational studies**
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- LXXIII. **A comprehensive and current review on the role of flavonoids in lung cancer–Experimental and theoretical approaches**
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- LXXIV. **Synthesis, spectral characterization, chemical reactivity and anticancer behaviors of some novel hydrazone derivatives: Experimental and theoretical insights**
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- LXXV. **One-Pot Hydrothermal Synthesized Nitrogen and Sulfur Codoped Carbon Dots for Acid Corrosion Inhibition of Q235 Steel br**
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- LXXVI. **Probing of Neural Networks as a Bridge from Ab Initio Relevant Characteristics to Differential Scanning Calorimetry Measurements of High-Energy Compounds**
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- LXXVII. **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**
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- LXXIX. **Novel gossypol-indole modification as a green corrosion inhibitor for low-carbon steel in aggressive alkaline-saline solution**
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- LXXX. **Suppressing inhibitory compounds by nanomaterials for highly efficient biofuel production: A review**
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- LXXXI. **Development of QSAR-based (MLR/ANN) predictive models for effective design of pyridazine corrosion inhibitors**
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- LXXXII. **Non-fullerene acceptor IDIC based on indacinodithiophene used as an electron donor for organic**

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LXXXIV. Experimental and DFT Modeling Studies for the Adsorptive Removal of Reactive Dyes from Wastewater

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LXXXV. Phenylamine/Amide Grafted in Silica as Sensing Nanocomposites for the Removal of Carbamazepine: A DFT Approach

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LXXXVI. An experimental and theoretical approach to electrochemical sensing of environmentally hazardous dihydroxy benzene isomers at polysorbate modified carbon paste electrode

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LXXXVII. Ab Initio Insight into the Interaction of Metal-Decorated Fluorinated Carbon Fullerenes with Anti-COVID Drugs

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

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

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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

Al-Otaibi J. S., Mary Y. S., Thomas R., KAYA S.

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

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

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XCIII. 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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- XCV. **Spectral studies and quantum chemical ab initio calculations for Copper(II) complexes of two heterocyclic aroylhydrazones**
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- XCVI. **Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives**
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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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- XCVIII. **Experimental and theoretical investigation on the inhibition performance of disulfide derivatives on cobalt corrosion in alkaline medium**
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- XCIX. **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**
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- C. **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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- CI. **Synthesis, identification, density functional and Hirshfeld surface studies of 2,2 '-disulfaneylbis(tetrahydro-4H-cyclopenta[d][1,3,2]dioxaphosphole-2-sulfide)**
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- CII. **Electrochemical investigations and theoretical studies of biocompatible niacin-modified carbon paste electrode interface for electrochemical sensing of folic acid**
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- CIII. **Papaver somniferum as an efficient corrosion inhibitor for iron alloy in acidic condition: DFT, MC simulation, LCMS and electrochemical studies**
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- CIV. **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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- CVI. **Molecular modelling of compounds used for corrosion inhibition studies: a review**
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- CVII. **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.
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- CVIII. **Quantum chemical studies and electrochemical investigations of pyrogallol red modified carbon paste electrode fabrication for sensor application**
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- CIX. **Decyltriphenylphosphonium bromide containing hydrophobic alkyl-chain as a potential corrosion inhibitor for mild steel in sulfuric acid: Theoretical and experimental studies**
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- CX. **Chemical characterization and evaluation of the neuroprotective potential of Indigofera sessiliflora through in-silico studies and behavioral tests in scopolamine-induced memory compromised rats**
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- CXI. **Investigation of plant waste as a renewable biomass source to develop efficient, economical and eco-friendly corrosion inhibitor**
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- CXII. **Zeolite/Cellulose Acetate (ZCA) in Blend Fiber for Adsorption of Erythromycin Residue From Pharmaceutical Wastewater: Experimental and Theoretical Study**
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- CXIII. **Corrosion inhibition, surface adsorption and computational studies of Swertia chirata extract: A sustainable and green approach**
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- CXIV. **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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- CXV. **Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries**
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- CXVI. **Thermo-magnetic properties of the screened Kratzer potential with spatially varying mass under the influence of Aharanov-Bohm(AB) and position-dependent magnetic fields**
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- CXVII. **Simulation and surface topology of activity of pyrazoloquinoline derivatives as corrosion inhibitor on the copper surfaces**
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- CXVIII. **Quantum Chemical Studies and Electrochemical Investigations of Polymerized Brilliant Blue-Modified Carbon Paste Electrode for In Vitro Sensing of Pharmaceutical Samples**
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- CXIX. **Investigations of Hg(II) analysis in real samples via computational chemistry, experimental design, and green microextraction approach**
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- CXX. **New imidazolium ionic liquids as ecofriendly corrosion inhibitors for mild steel in hydrochloric acid**

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- CXXI. **Adsorption of Eriochrome Black T on the chitin surface: Experimental study, DFT calculations and molecular dynamics simulation**
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- CXXII. **Diversities in the chelation of aroylhydrazones towards cobalt(II) salts: Synthesis, spectral characterization, crystal structure and some theoretical studies**
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- CXXIII. **Hydroxy phenyl hydrazides and their role as corrosion impeding agent: A detail experimental and theoretical study**
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- CXXIV. **Investigations on some coumarin based corrosion inhibitors for mild steel in aqueous acidic medium: Electrochemical, surface morphological, density functional theory and Monte Carlo simulation approach**
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- CXXV. **Ab initio Study of Hydrogen Adsorption on Metal-Decorated Borophene-Graphene Bilayer**
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- CXXVI. **Optimization of an ultrasound-assisted alcohol-based deep eutectic solvent dispersive liquid-phase microextraction for separation and preconcentration of quercetin in wine and food samples with response surface methodology**
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- CXXVII. **Theoretical computation of normalised radii, density and global hardness as a function of orbital exponent**
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- CXXVIII. **Sodium nitrite as a corrosion inhibitor of copper in simulated cooling water**
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- CXXIX. **Solutions of the 2D Schrodinger equation and its thermal properties for improved ultra-generalized exponential hyperbolic potential (IUGE-HP)**
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- CXXX. **Illuminating of mild steel/HCl interface in the presence of 5-DAT inhibitor**
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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_{0.4}Sb_{0.6}/In_{0.7}Ga_{0.3}As/GaAs_{0.4}Sb_{0.6} nano-heterostructure under electric field and [100] strain**
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- CXXXIII. **Experimental and theoretical study of new Schiff bases based on imidazo(1,2-a)pyridine as corrosion inhibitor of mild steel in 1M HCl**
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- CXXXIV. **Insights into corrosion inhibition mechanism of mild steel in 1 M HCl solution by quinoxaline derivatives: electrochemical, SEM/EDAX, UV-visible, FT-IR and theoretical approaches**
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- CXXXV. **A combined molecular dynamic simulation, DFT calculations, and experimental study of the eriochrome black T dye adsorption onto chitosan in aqueous solutions**
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- CXXXVI. **Equilibrium, thermodynamic, and density functional theory modeling studies for the removal of dichromate ions from wastewater using calix[4]arene modified silica resin**
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- CXXXVII. **Synthesis, crystal structure, hirshfeld surface analysis, spectroscopic, biological and first-principles studies of novel aminocoumarins**
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- CXXXVIII. **Spectrophotometric determination of aflatoxin B1 in food sample: Chemometric optimization and theoretical supports for reaction mechanisms and binding regions**
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- CXXXIX. **Eco-friendly sodium gluconate and trisodium citrate inhibitors for low carbon steel in simulated cooling water system: Theoretical study and molecular dynamic simulations**
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- CXL. **Why and When Is Electrophilicity Minimized? New Theorems and Guiding Rules**
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- CXLI. **Evaluation of inhibitive and adsorption behavior of thiazole-4-carboxylates on mild steel corrosion in HCl**
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- CXLII. **Aminoantipyrine derivatives as a novel eco-friendly corrosion inhibitors for P110 steel in simulating acidizing environment: Experimental and computational studies**
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- CXLIII. **Synthesis, experimental and theoretical characterization of (E)-2-((2,3-dimethylphenyl)amino)-N'-(furan-2-ylmethylene) benzohydrazide**
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- CXLIV. **Theoretical insights about inhibition efficiencies of some 8-Hydroxyqionoline derivatives against the corrosion of mild steel**
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- CXLV. **Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies**

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- CXLVI. **Spectroscopic studies, molecular structure optimization and investigation of structural and electrical properties of novel and biodegradable Chitosan-GO polymer nanocomposites**
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- CXLVII. **Mixed ligand copper(II) chelates derived from an O, N, S- donor tridentate thiosemicarbazone: Synthesis, spectral aspects, FMO, and NBO analysis**
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- CXLVIII. **Interaction of dopants and functional groups adsorbed on the carbon fullerenes: Computational study**
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- CLI. **Effective Removal of the Direct Black-38 Dye from Wastewater Using a New Silica-Modified Resin: Equilibrium and Thermodynamics Modeling Studies**
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- CLII. **Electrochemical and Computational Investigations on the Corrosion Inhibition of X65 Steel by 2-Phenylbenzimidazole in H2SO4 Solution**
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- CLIII. **Insight from adsorption properties of Xylidyl Blue embedded hydrogel for effective removal of uranyl: Experimental and theoretical approaches**
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- CLV. **Cyclotriphosphazene based dendrimeric epoxy resin as an anti-corrosive material for copper in 3% NaCl: Experimental and computational demonstrations**
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- CLVIII. **Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculations of 2-[(2,3-dimethylphenyl)amino]-N'-(E)-thiophen-2-ylmethylidene]benzohydrazide**
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- I. **Evaluation of the interactions of the Sunitinib malate with topoisomerase enzymes by in vitro**

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