

Tuhin Suvra Khan

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5309594/publications.pdf>

Version: 2024-02-01

62
papers

1,939
citations

257450

24
h-index

265206

42
g-index

62
all docs

62
docs citations

62
times ranked

2242
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine Learning Enabled Screening of Single Atom Alloys: Predicting Reactivity Trend for Ethanol Dehydrogenation. <i>ChemCatChem</i> , 2022, 14, .	3.7	13
2	Single-step synthesis of 2-pentanone from furfural over Cu@Ni @SBA-15. <i>Biomass and Bioenergy</i> , 2022, 156, 106321.	5.7	9
3	Highly regenerative, fast colorimetric response for organo-toxin and oxo-anions in an aqueous medium using a discrete luminescent Cd(L) complex in a heterogeneous manner with theoretical revelation. <i>Dalton Transactions</i> , 2022, 51, 7436-7454.	3.3	9
4	Understanding Na-Ion Transport in Na ₂ V ₄ O ₁₀ Electrode Material for Sodium-Ion Batteries. <i>Journal of Electronic Materials</i> , 2021, 50, 1794-1799.	2.2	6
5	CO ₂ reduction and ethane dehydrogenation on transition metal catalysts: mechanistic insights, reactivity trends and rational design of bimetallic alloys. <i>Catalysis Science and Technology</i> , 2021, 11, 97-115.	4.1	18
6	Unravelling the reactivity of metastable molybdenum carbide nanoclusters in the C-H bond activation of methane, ethane and ethylene. <i>Nanoscale</i> , 2021, 13, 4451-4466.	5.6	6
7	Activation of two highly stable molecules – nitrogen and methane to co-produce ammonia and ethylene. <i>Chemical Engineering Journal</i> , 2021, 413, 127501.	12.7	8
8	Understanding the origin of structure sensitivity in hydrodechlorination of trichloroethylene on a palladium catalyst. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 2270-2279.	3.7	3
9	Catalytic decomposition of methane into hydrogen and high-value carbons: combined experimental and DFT computational study. <i>Catalysis Science and Technology</i> , 2021, 11, 4911-4921.	4.1	24
10	Supersensitive Detection of Anions in Pure Organic and Aqueous Media by Amino Acid Conjugated Ellman's Reagent. <i>ACS Applied Bio Materials</i> , 2021, 4, 2453-2464.	4.6	6
11	Insights into the activity and selectivity trends in non-oxidative dehydrogenation of primary and secondary alcohols over the copper catalyst. <i>Catalysis Today</i> , 2021, 370, 151-160.	4.4	17
12	Understanding the Origin of Structure Sensitivity in Nano Crystalline Mixed Cu/Mg ²⁺ Al Oxides Catalyst for Low-Pressure Methanol Synthesis. <i>ChemCatChem</i> , 2021, 13, 3290-3302.	3.7	8
13	Selective transfer hydrogenation of biomass derived furanic molecules using cyclohexanol as a hydrogen donor over nanostructured Cu/MgO catalyst. <i>Molecular Catalysis</i> , 2021, 513, 111812.	2.0	8
14	Design of highly stable MgO promoted Cu/ZnO catalyst for clean methanol production through selective hydrogenation of CO ₂ . <i>Applied Catalysis A: General</i> , 2021, 623, 118239.	4.3	40
15	In-situ experimental and computational approach to investigate the nature of active site in low-temperature CO-PROX over CuOx-CeO ₂ catalyst. <i>Applied Catalysis A: General</i> , 2021, 624, 118305.	4.3	20
16	Direct Oxidation of Cyclohexane to Adipic Acid by a WFeCoO(OH) Catalyst: Role of Brønsted Acidity and Oxygen Vacancies. <i>ACS Catalysis</i> , 2021, 11, 10754-10766.	11.2	29
17	Exploring bimetallic alloy catalysts of Co, Pd and Cu for CO ₂ reduction combined with ethane dehydrogenation. <i>Applied Energy</i> , 2021, 299, 117284.	10.1	7
18	Microwave-enhanced catalytic ammonia synthesis under moderate pressure and temperature. <i>Catalysis Communications</i> , 2021, 159, 106344.	3.3	14

#	ARTICLE	IF	CITATIONS
19	CuO as a reactive and reusable reagent for the hydrogenation of nitroarenes. Applied Catalysis B: Environmental, 2021, 297, 120417.	20.2	32
20	Thermocatalytic Conversion of Natural Gas to Petrochemical Feedstocks Via Non-oxidative Methods: Theoretical and Experimental Approaches. , 2021, , 229-252.		0
21	Mechanistic insights into the dominant reaction route and catalyst deactivation in biogas reforming using <i>ab initio</i> microkinetic modeling. Catalysis Science and Technology, 2021, 11, 2130-2143.	4.1	14
22	Graphene-Supported Fe/Ni, γ -Mo ₂ C Nanoparticles: Experimental and DFT Integrated Approach to Catalyst Development for Synergistic Hydrogen Production through Lignin-Rich Biomass Reforming and Reduced Shale Gas Flaring. ACS Catalysis, 2021, 11, 364-382.	11.2	9
23	Tracing the reactivity of single atom alloys for ethanol dehydrogenation using <i>ab initio</i> simulations. Reaction Chemistry and Engineering, 2021, 7, 61-75.	3.7	4
24	The Operating Cycle of NO Adsorption and Desorption in Pd ^{δ+} Chabazite for Passive NO _x Adsorbers. Langmuir, 2021, 37, 13799-13809.	3.5	10
25	Role of Interfacial Cu ^{δ+} ions in Polycrystalline Cu ^{δ+} CeO ₂ : In ^{δ+} situ Raman, In ^{δ+} situ DRIFT and DFT Studies for Preferential Oxidation of CO in Presence of Excess H ₂ **. ChemistrySelect, 2021, 6, 13051-13059.	1.5	7
26	<i>In silico</i> high throughput screening of bimetallic and single atom alloys using machine learning and <i>ab initio</i> microkinetic modelling. Journal of Materials Chemistry A, 2020, 8, 107-123.	10.3	48
27	Mechanistic Elucidation of Surface Cation Segregation in Double Perovskite PrBaCo ₂ O ₅ + δ Material using MD and DFT Simulations for Solid Oxide Fuel Cells. Ionics, 2020, 26, 1307-1314.	2.4	9
28	Diffusion coefficient and electrochemical performance of NaVO ₃ anode in Li/Na batteries. Electrochimica Acta, 2020, 331, 135293.	5.2	48
29	Effect of substituents and promoters on the Diels-Alder cycloaddition reaction in the biorenewable synthesis of trimellitic acid. RSC Advances, 2020, 10, 30656-30670.	3.6	11
30	Understanding reaction kinetics, deprotonation and solvation of Brønsted acidic protons in heteropolyacid catalyzed synthesis of biorenewable alkyl levulinates. Chemical Engineering Journal, 2020, 400, 125916.	12.7	41
31	Boric acid treated HZSM-5 for improved catalyst activity in non-oxidative methane dehydroaromatization. Catalysis Science and Technology, 2020, 10, 3857-3867.	4.1	22
32	Utility of Silver Nanoparticles Embedded Covalent Organic Frameworks as Recyclable Catalysts for the Sustainable Synthesis of Cyclic Carbamates and 2-Oxazolidinones via Atmospheric Cyclizative CO ₂ Capture. ACS Sustainable Chemistry and Engineering, 2020, 8, 5495-5513.	6.7	73
33	Elucidating the role of solvents in acid catalyzed dehydration of biorenewable hydroxy-lactones. Reaction Chemistry and Engineering, 2020, 5, 651-662.	3.7	7
34	Spectroscopic Evidences for the Size Dependent Generation of Pd Species Responsible for the Low Temperature CO Oxidation Activity on Pd-SBA-15 Nanocatalyst. Applied Catalysis B: Environmental, 2020, 272, 118934.	20.2	31
35	Identifying the Origin of the Limiting Process in a Double Perovskite PrBa _{0.5} Sr _{0.5} Co _{1.5} Fe _{0.5} O _{5+δ} Thin-Film Electrode for Solid Oxide Fuel Cells. ACS Applied Materials & Interfaces, 2019, 11, 25243-25253.	8.0	23
36	Mechanistic Insights into the Pathways of Phenol Hydrogenation on Pd Nanostructures. ACS Sustainable Chemistry and Engineering, 2019, 7, 17126-17136.	6.7	57

#	ARTICLE	IF	CITATIONS
37	Electrochemical Properties of $\text{Na}_{0.66}\text{V}_4\text{O}_{10}$ Nanostructures as Cathode Material in Rechargeable Batteries for Energy Storage Applications. <i>ACS Omega</i> , 2019, 4, 9878-9888.	3.5	15
38	Mechanistic Approaches toward Rational Design of a Heterogeneous Catalyst for Ring-Opening and Deoxygenation of Biomass-Derived Cyclic Compounds. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 10165-10181.	6.7	30
39	Synergistic Effect of Zn in a Bimetallic PdZn Catalyst: Elucidating the Role of Undercoordinated Sites in the Hydrodeoxygenation Reactions of Biorenewable Platforms. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 16153-16163.	3.7	22
40	In-silico screening of Pt-based bimetallic alloy catalysts using ab initio microkinetic modeling for non-oxidative dehydrogenation of ethanol to produce acetaldehyde. <i>MRS Communications</i> , 2019, 9, 107-113.	1.8	10
41	Controlling surface cation segregation in a nanostructured double perovskite $\text{GdBaCo}_2\text{O}_{5+\delta}$ electrode for solid oxide fuel cells. <i>Nanoscale</i> , 2019, 11, 21404-21418.	5.6	24
42	Alternate Biobased Route To Produce γ -Decalactone: Elucidating the Role of Solvent and Hydrogen Evolution in Catalytic Transfer Hydrogenation. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 2894-2898.	6.7	29
43	Understanding the Nature of Amino Acid Interactions with Pd(111) or Pd-Au Bimetallic Catalysts in the Aqueous Phase. <i>Langmuir</i> , 2018, 34, 1300-1310.	3.5	10
44	On the role of oxocarbenium ions formed in Brønsted acidic condition on $\gamma\text{-Al}_2\text{O}_3$ surface in the ring-opening of β -valerolactone. <i>Applied Catalysis A: General</i> , 2018, 560, 66-72.	4.3	18
45	In-silico screening of metal and bimetallic alloy catalysts for SOFC anode at high, intermediate and low temperature operations. <i>Electrochimica Acta</i> , 2018, 281, 654-664.	5.2	13
46	Mechanistic Insights into the Activity of Mo-Carbide Clusters for Methane Dehydrogenation and Carbon-Carbon Coupling Reactions To Form Ethylene in Methane Dehydroaromatization. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11754-11764.	3.1	29
47	A Car-Parrinello Molecular Dynamics Simulation Study of the Retro Diels-Alder Reaction for Partially Saturated 2-Pyrones in Water. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11599-11607.	3.1	11
48	First-Principle Microkinetic Modeling of Ethanol Dehydrogenation on Metal Catalyst Surfaces in Non-oxidative Environment: Design of Bimetallic Alloys. <i>Topics in Catalysis</i> , 2018, 61, 1820-1831.	2.8	27
49	Acid functionalized ionic liquid catalyzed transformation of non-food biomass into platform chemical and fuel additive. <i>Industrial Crops and Products</i> , 2018, 123, 629-637.	5.2	49
50	Effect of Fe-Doping on Oxygen Anion Diffusion in $\text{PrBaCo}_{2-x}\text{Fe}_x\text{O}_{5+\delta}$ Double Perovskite Electrodes for Solid Oxide Fuel Cells. <i>ECS Transactions</i> , 2017, 77, 125-131.	0.5	6
51	Ca-Doped Double Perovskite $\text{PrBa}_{0.8}\text{Ca}_{0.2}\text{Co}_2\text{O}_{5+\delta}$ Thin-Film Electrodes: Experimental and Theoretical Study. <i>ECS Transactions</i> , 2017, 78, 499-506.	0.5	2
52	Understanding trends in hydrodeoxygenation reactivity of metal and bimetallic alloy catalysts from ethanol reaction on stepped surface. <i>Journal of Catalysis</i> , 2017, 353, 265-273.	6.2	46
53	Non-bonding and bonding interactions of biogenic impurities with the metal catalyst and the design of bimetallic alloys. <i>Journal of Catalysis</i> , 2017, 352, 542-556.	6.2	13
54	Reformulation of Gasoline To Replace Aromatics by Biomass-Derived Alkyl Levulinates. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 7118-7127.	6.7	33

#	ARTICLE	IF	CITATIONS
55	Development of 6-acyl- γ -pyrone as a potential biomass-derived platform molecule. <i>Green Chemistry</i> , 2016, 18, 6431-6435.	9.0	41
56	Reactivity descriptor for the retro Diels-Alder reaction of partially saturated 2-pyrone: DFT study on substituents and solvent effects. <i>RSC Advances</i> , 2016, 6, 101697-101706.	3.6	28
57	On the mechanism of retro-Diels-Alder reaction of partially saturated 2-pyrone to produce biorenewable chemicals. <i>RSC Advances</i> , 2016, 6, 60433-60445.	3.6	26
58	On the role of the surface oxygen species during A-H (A = C, N, O) bond activation: a density functional theory study. <i>Chemical Communications</i> , 2015, 51, 2621-2624.	4.1	51
59	Exploring the limits: A low-pressure, low-temperature Haber-Bosch process. <i>Chemical Physics Letters</i> , 2014, 598, 108-112.	2.6	369
60	On the Structure Sensitivity of Direct NO Decomposition over Low-Index Transition Metal Facets. <i>Topics in Catalysis</i> , 2014, 57, 80-88.	2.8	64
61	On the effect of coverage-dependent adsorbate-adsorbate interactions for CO methanation on transition metal surfaces. <i>Journal of Catalysis</i> , 2013, 307, 275-282.	6.2	217
62	<i>In silico</i> search for novel methane steam reforming catalysts. <i>New Journal of Physics</i> , 2013, 15, 125021.	2.9	65