Tuhin Suvra Khan

List of Publications by Year
in descending order

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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	Exploring the limits: A low-pressure, low-temperature Haberâ€“Bosch process. Chemical Physics Letters, 2014, 598, 108-112.	2.6	369
2	On the effect of coverage-dependent adsorbateâ€“adsorbate interactions for CO methanation on transition metal surfaces. Journal of Catalysis, 2013, 307, 275-282.	6.2	217
3	Utility of Silver Nanoparticles Embedded Covalent Organic Frameworks as Recyclable Catalysts for the Sustainable Synthesis of Cyclic Carbamates and 2-Oxazolidinones via Atmospheric Cyclizative CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2020, 8, 5495-5513.	6.7	73
4	In silicosearch for novel methane steam reforming catalysts. New Journal of Physics, 2013, 15, 125021.	2.9	65
5	On the Structure Sensitivity of Direct NO Decomposition over Low-Index Transition Metal Facets. Topics in Catalysis, 2014, 57, 80-88.	2.8	64
6	Mechanistic Insights into the Pathways of Phenol Hydrogenation on Pd Nanostructures. ACS Sustainable Chemistry and Engineering, 2019, 7, 17126-17136.	6.7	57
7	On the role of the surface oxygen species during Aâ€“H (A = C, N, O) bond activation: a density functional theory study. Chemical Communications, 2015, 51, 2621-2624.	4.1	51
8	Acid functionalized ionic liquid catalyzed transformation of non-food biomass into platform chemical and fuel additive. Industrial Crops and Products, 2018, 123, 629-637.	5.2	49
9	In silicohigh throughput screening of bimetallic and single atom alloys using machine learning andab initiomicrokinetic modelling. Journal of Materials Chemistry A, 2020, 8, 107-123.	10.3	48
10	Diffusion coefficient and electrochemical performance of NaVO3 anode in Li/Na batteries. Electrochimica Acta, 2020, 331, 135293.	5.2	48
11	Understanding trends in hydrodeoxygenation reactivity of metal and bimetallic alloy catalysts from ethanol reaction on stepped surface. Journal of Catalysis, 2017, 353, 265-273.	6.2	46
12	Development of 6-amyl-Î±-pyrone as a potential biomass-derived platform molecule. Green Chemistry, 2016, 18, 6431-6435.	9.0	41
13	Understanding reaction kinetics, deprotonation and solvation of brÃ¸nsted acidic protons in heteropolyacid catalyzed synthesis of biorenewable alkyl levulinates. Chemical Engineering Journal, 2020, 400, 125916.	12.7	41
14	Design of highly stable MgO promoted Cu/ZnO catalyst for clean methanol production through selective hydrogenation of CO2. Applied Catalysis A: General, 2021, 623, 118239.	4.3	40
15	Reformulation of Gasoline To Replace Aromatics by Biomass-Derived Alkyl Levulinates. ACS Sustainable Chemistry and Engineering, 2017, 5, 7118-7127.	6.7	33
16	CuO as a reactive and reusable reagent for the hydrogenation of nitroarenes. Applied Catalysis B: Environmental, 2021, 297, 120417.	20.2	32
17	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
18	Mechanistic Approaches toward Rational Design of a Heterogeneous Catalyst for Ring-Opening and Deoxygenation of Biomass-Derived Cyclic Compounds. ACS Sustainable Chemistry and Engineering, 2019, 7, 10165-10181.	6.7	30

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19	Mechanistic Insights into the Activity of Mo-Carbide Clusters for Methane Dehydrogenation and Carbonâ€“Carbon Coupling Reactions To Form Ethylene in Methane Dehydroaromatization. Journal of Physical Chemistry C, 2018, 122, 11754-11764.	3.1	29
20	Alternate Biobased Route To Produce Î´-Decalactone: Elucidating the Role of Solvent and Hydrogen Evolution in Catalytic Transfer Hydrogenation. ACS Sustainable Chemistry and Engineering, 2019, 7, 2894-2898.	6.7	29
21	Direct Oxidation of Cyclohexane to Adipic Acid by a WFeCoO(OH) Catalyst: Role of BrÃ¸nsted Acidity and Oxygen Vacancies. ACS Catalysis, 2021, 11, 10754-10766.	11.2	29
22	Reactivity descriptor for the retro Dielsâ€“Alder reaction of partially saturated 2-pyrones: DFT study on substituents and solvent effects. RSC Advances, 2016, 6, 101697-101706.	3.6	28
23	First-Principle Microkinetic Modeling of Ethanol Dehydrogenation on Metal Catalyst Surfaces in Non-oxidative Environment: Design of Bimetallic Alloys. Topics in Catalysis, 2018, 61, 1820-1831.	2.8	27
24	On the mechanism of retro-Dielsâ€“Alder reaction of partially saturated 2-pyrones to produce biorenewable chemicals. RSC Advances, 2016, 6, 60433-60445.	3.6	26
25	Controlling surface cation segregation in a nanostructured double perovskite GdBaCo₂O_{5+Î´} electrode for solid oxide fuel cells. Nanoscale, 2019, 11, 21404-21418.	5.6	24
26	Catalytic decomposition of methane into hydrogen and high-value carbons: combined experimental and DFT computational study. Catalysis Science and Technology, 2021, 11, 4911-4921.	4.1	24
27	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+Î´} Thin-Film Electrode for Solid Oxide Fuel Cells. ACS Applied Materials & Interfaces, 2019, 11, 25243-25253.	8.0	23
28	Synergistic Effect of Zn in a Bimetallic PdZn Catalyst: Elucidating the Role of Undercoordinated Sites in the Hydrodeoxygenation Reactions of Biorenewable Platforms. Industrial & Engineering Chemistry Research, 2019, 58, 16153-16163.	3.7	22
29	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
30	In-situ experimental and computational approach to investigate the nature of active site in low-temperature CO-PROX over CuOx-CeO2 catalyst. Applied Catalysis A: General, 2021, 624, 118305.	4.3	20
31	On the role of oxocarbenium ions formed in BrÃ¸nsted acidic condition on Î³-Al2O3 surface in the ring-opening of Î³-valerolactone. Applied Catalysis A: General, 2018, 560, 66-72.	4.3	18
32	CO₂ reduction and ethane dehydrogenation on transition metal catalysts: mechanistic insights, reactivity trends and rational design of bimetallic alloys. Catalysis Science and Technology, 2021, 11, 97-115.	4.1	18
33	Insights into the activity and selectivity trends in non-oxidative dehydrogenation of primary and secondary alcohols over the copper catalyst. Catalysis Today, 2021, 370, 151-160.	4.4	17
34	Electrochemical Properties of Na_{0.66}V₄O₁₀ Nanostructures as Cathode Material in Rechargeable Batteries for Energy Storage Applications. ACS Omega, 2019, 4, 9878-9888.	3.5	15
35	Microwave-enhanced catalytic ammonia synthesis under moderate pressure and temperature. Catalysis Communications, 2021, 159, 106344.	3.3	14
36	Mechanistic insights into the dominant reaction route and catalyst deactivation in biogas reforming using ab initio microkinetic modeling. Catalysis Science and Technology, 2021, 11, 2130-2143.	4.1	14

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37	Non-bonding and bonding interactions of biogenic impurities with the metal catalyst and the design of bimetallic alloys. Journal of Catalysis, 2017, 352, 542-556.	6.2	13
38	In-silico screening of metal and bimetallic alloy catalysts for SOFC anode at high, intermediate and low temperature operations. Electrochimica Acta, 2018, 281, 654-664.	5.2	13
39	Machine Learning Enabled Screening of Single Atom Alloys: Predicting Reactivity Trend for Ethanol Dehydrogenation. ChemCatChem, 2022, 14, .	3.7	13
40	A Carâ€“Parrinello Molecular Dynamics Simulation Study of the Retro Dielsâ€“Alder Reaction for Partially Saturated 2-Pyrones in Water. Journal of Physical Chemistry C, 2018, 122, 11599-11607.	3.1	11
41	Effect of substituents and promoters on the Dielsâ€“Alder cycloaddition reaction in the biorenewable synthesis of trimellitic acid. RSC Advances, 2020, 10, 30656-30670.	3.6	11
42	Understanding the Nature of Amino Acid Interactions with Pd(111) or Pdâ€“Au Bimetallic Catalysts in the Aqueous Phase. Langmuir, 2018, 34, 1300-1310.	3.5	10
43	In-silico screening of Pt-based bimetallic alloy catalysts using ab initio microkinetic modeling for non-oxidative dehydrogenation of ethanol to produce acetaldehyde. MRS Communications, 2019, 9, 107-113.	1.8	10
44	The Operating Cycle of NO Adsorption and Desorption in Pdâ€“Chabazite for Passive NO_x Adsorbers. Langmuir, 2021, 37, 13799-13809.	3.5	10
45	Mechanistic Elucidation of Surface Cation Segregation in Double Perovskite PrBaCo2O5+Î´ Material using MD and DFT Simulations for Solid Oxide Fuel Cells. Ionics, 2020, 26, 1307-1314.	2.4	9
46	Graphene-Supported Fe/Ni, Î²-Mo2C 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
47	Single-step synthesis of 2-pentanone from furfural over Cuâ€“Ni @SBA-15. Biomass and Bioenergy, 2022, 156, 106321.	5.7	9
48	Highly regenerative, fast colorimetric response for organo-toxin and oxo-anions in an aqueous medium using a discrete luminescent Cd(<scp>ii</scp>) complex in a heterogeneous manner with theoretical revelation. Dalton Transactions, 2022, 51, 7436-7454.	3.3	9
49	Activation of two highly stable molecules â€“ nitrogen and methane to co-produce ammonia and ethylene. Chemical Engineering Journal, 2021, 413, 127501.	12.7	8
50	Understanding the Origin of Structure Sensitivity in Nano Crystalline Mixed Cu/Mgâ^'Al Oxides Catalyst for Lowâ€Pressure Methanol Synthesis. ChemCatChem, 2021, 13, 3290-3302.	3.7	8
51	Selective transfer hydrogenation of biomass derived furanic molecules using cyclohexanol as a hydrogen donor over nanostructured Cu/MgO catalyst. Molecular Catalysis, 2021, 513, 111812.	2.0	8
52	Elucidating the role of solvents in acid catalyzed dehydration of biorenewable hydroxy-lactones. Reaction Chemistry and Engineering, 2020, 5, 651-662.	3.7	7
53	Exploring bimetallic alloy catalysts of Co, Pd and Cu for CO2 reduction combined with ethane dehydrogenation. Applied Energy, 2021, 299, 117284.	10.1	7
54	Role of Interfacial Cuâ€Ions in Polycrystalline Cuâ€CeO 2 : Inâ€Situ Raman, Inâ€situ DRIFT and DFT Studies for Preferential Oxidation of CO in Presence of Excess H 2 **. ChemistrySelect, 2021, 6, 13051-13059.	1.5	7

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55	Effect of Fe-Doping on Oxygen Anion Diffusion in PrBaCo _{2-x} Fe _x O _{5+Î´} Double Perovskite Electrodes for Solid Oxide Fuel Cells. ECS Transactions, 2017, 77, 125-131.	0.5	6
56	Understanding Na-Ion Transport in NaxV4O10 Electrode Material for Sodium-Ion Batteries. Journal of Electronic Materials, 2021, 50, 1794-1799.	2.2	6
57	Unravelling the reactivity of metastable molybdenum carbide nanoclusters in the Câ€“H bond activation of methane, ethane and ethylene. Nanoscale, 2021, 13, 4451-4466.	5.6	6
58	Supersensitive Detection of Anions in Pure Organic and Aqueous Media by Amino Acid Conjugated Ellmanâ€™s Reagent. ACS Applied Bio Materials, 2021, 4, 2453-2464.	4.6	6
59	Tracing the reactivity of single atom alloys for ethanol dehydrogenation using ab initio simulations. Reaction Chemistry and Engineering, 2021, 7, 61-75.	3.7	4
60	Understanding the origin of structure sensitivity in hydrodechlorination of trichloroethylene on a palladium catalyst. Reaction Chemistry and Engineering, 2021, 6, 2270-2279.	3.7	3
61	Ca-Doped Double Perovskite PrBa_{0.8}Ca_{0.2}Co₂O_{5+Î´}Thin-Film Electrodes: Experimental and Theoretical Study. ECS Transactions, 2017, 78, 499-506.	0.5	2
62	Thermocatalytic Conversion of Natural Gas to Petrochemical Feedstocks Via Non-oxidative Methods: Theoretical and Experimental Approaches. , 2021, , 229-252.		0