Talat S Rahman

List of Publications by Year
in descending order

133 papers	3,697 citations	159358 30 h-index	155451 55 g-index
136 all docs	136 docs citations	136 times ranked	4549 citing authors

#	Article	IF	Citations
1	Methanol carbonylation to acetaldehyde on Au particles supported by single-layer MoS₂ grown on silica. Journal of Physics Condensed Matter, 2022, 34, 104005.	0.7	1
2	Atomic and molecular functionalisation of technological materials: an introduction to nanoscale processes on semiconductor surfaces. Journal of Physics Condensed Matter, 2022, 34, 210401.	0.7	0
3	Defect engineering of oxide surfaces: dream or reality?. Journal of Physics Condensed Matter, 2022, 34, 291501.	0.7	2
4	Nonadiabatic Exchange-Correlation Potential for Strongly Correlated Materials in the Weak and Strong Interaction Limits. Computation, 2022, 10, 77.	1.0	0
5	Nonmetal-to-Metal Transition of Magnesia Supported Au Clusters Affects the Ultrafast Dissociation Dynamics of Adsorbed CH₃Br Molecules. Journal of Physical Chemistry Letters, 2022, 13, 4747-4753.	2.1	1
6	Ligand-coordination effects on the selective hydrogenation of acetylene in single-site Pd-ligand supported catalysts. Journal of Catalysis, 2022, 413, 81-92.	3.1	8
7	Syngas molecules as probes for defects in 2D hexagonal boron nitride: their adsorption and vibrations. Physical Chemistry Chemical Physics, 2021, 23, 7988-8001.	1.3	9
8	Ultrafast charge dynamics and photoluminescence in bilayer MoS₂. 2D Materials, 2021, 8, 025018.	2.0	7
9	Electron thermalization and relaxation in laser-heated nickel by few-femtosecond core-level transient absorption spectroscopy. Physical Review B, 2021, 103, .	1.1	21
10	Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride. ACS Sustainable Chemistry and Engineering, 2021, 9, 2447-2455.	3.2	25
11	Fermi surfaces of the topological semimetal CaSn₃ probed through de Haas van Alphen oscillations. Journal of Physics Condensed Matter, 2021, 33, 17LT01.	0.7	4
12	Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS2 â€“ predictions from DFT+KMC. Journal of Chemical Physics, 2021, 154, 174701.	1.2	3
13	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. Physical Review B, 2021, 103, .	1.1	1
14	On stabilizing spin crossover molecule [Fe(tBu₂qsal)₂] on suitable supports: insights from ab initio studies. Journal of Physics Condensed Matter, 2021, 33, 385201.	0.7	1
15	Anisotropic Properties of Quasiâ€1D In₄Se₃: Mechanical Exfoliation, Electronic Transport, and Polarizationâ€Dependent Photoresponse. Advanced Functional Materials, 2021, 31, 2106459.	7.8	11
16	Asymmetric Design of Spin-Crossover Complexes to Increase the Volatility for Surface Deposition. Journal of the American Chemical Society, 2021, 143, 14563-14572.	6.6	16
17	Growth of Graphene Nanoflakes/hâ€BN Heterostructures. Advanced Materials Interfaces, 2021, 8, 2100766.	1.9	5
18	Tailoring the redox capabilities of organic ligands for metal-ligand coordination with vanadium single-sites. Surface Science, 2021, 712, 121888.	0.8	1

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19	Excited states in hydrogenated single-layer MoS₂. Journal of Physics Condensed Matter, 2021, 33, 075201.	0.7	0
20	Anisotropy-exchange resonance as a mechanism for entangled state switching. Physical Review A, 2021, 104, .	1.0	6
21	Atomic-Scale Structure and Catalysis on Positively Charged Bimetallic Sites for Generation of H₂. Nano Letters, 2020, 20, 6255-6262.	4.5	10
22	Characteristics of Single-Molecule Magnet Dimers ([Mn₃]₂) on Graphene and h-BN. Journal of Physical Chemistry C, 2020, 124, 28186-28200.	1.5	11
23	MoS2-supported Au31 for CO hydrogenation: A first-principle study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, 032201.	0.9	0
24	Plasmon excitations in chemically heterogeneous nanoarrays. Physical Review B, 2020, 101, .	1.1	11
25	Catalytic C2H2 synthesis via low temperature CO hydrogenation on defect-rich 2D-MoS2 and 2D-MoS2 decorated with Mo clusters. Journal of Chemical Physics, 2020, 152, 074706.	1.2	3
26	Ultrafast Electron Correlations and Memory Effects at Work: Femtosecond Demagnetization in Ni. Physical Review Letters, 2020, 125, 017202.	2.9	35
27	Metallicity of 2H-MoS₂ induced by Au hybridization. 2D Materials, 2020, 7, 025021.	2.0	17
28	CO Oxidation Mechanisms on CoO_x-Pt Thin Films. Journal of the American Chemical Society, 2020, 142, 8312-8322.	6.6	39
29	Dominant contributions to the apparent activation energy in two-dimensional submonolayer growth: comparison between Cu/Ni(111) and Ni/Cu(111). Journal of Physics Condensed Matter, 2020, 32, 445002.	0.7	1
30	Surface Thermodynamics and Vibrational Entropy. Springer Handbooks, 2020, , 71-93.	0.3	2
31	Self-Catalyzed, Low-Temperature Atomic Layer Deposition of Ruthenium Metal Using Zero-Valent Ru(DMBD)(CO)₃ and Water. Chemistry of Materials, 2019, 31, 1304-1317.	3.2	20
32	Effects of Î³-Al2O3 Support on the Morphology and Electronic Structure of Pt Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 16893-16901.	1.5	7
33	Analysis of the fluorescence of mechanically processed defect-laden hexagonal boron nitride and the role of oxygen in catalyst deactivation. Advances in Applied Ceramics, 2019, 118, 153-158.	0.6	5
34	MoS₂ Nanoclusters Grown on TiO₂: Evidence for New Adsorption Sites at Edges and Sulfur Vacancies. Journal of Physical Chemistry C, 2019, 123, 7185-7201.	1.5	18
35	Plasmon Excitations in Mixed Metallic Nanoarrays. ACS Nano, 2019, 13, 5344-5355.	7.3	21
36	Multiâ€electron Reduction Capacity and Multiple Binding Pockets in Metalâ€“Organic Redox Assembly at Surfaces. Chemistry - A European Journal, 2019, 25, 5565-5573.	1.7	7

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37	A Single Layer of MoS2 Activates Gold for Room Temperature CO Oxidation on an Inert Silica Substrate. Journal of Physical Chemistry C, 2019, 123, 6592-6598.	1.5	11
38	Toward multiscale modeling of thin-film growth processes using SLKMC. Journal of Materials Research, 2018, 33, 709-719.	1.2	5
39	Methoxy Formation Induced Defects on MoS₂. Journal of Physical Chemistry C, 2018, 122, 10042-10049.	1.5	11
40	Redox-active ligand controlled selectivity of vanadium oxidation on Au(100). Chemical Science, 2018, 9, 1674-1685.	3.7	24
41	Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS₂. Journal of Physical Chemistry C, 2018, 122, 267-273.	1.5	16
42	Deciphering complex features in STM images of O adatoms on Ag(110). Physical Review B, 2018, 98, .	1.1	6
43	Redox Isomeric Surface Structures Are Preferred over Oddâ€Electron Pt 1+. Chemistry - A European Journal, 2018, 24, 15852-15858.	1.7	7
44	Effect of Single-Layer MoS₂ on the Geometry, Electronic Structure, and Reactivity of Transition Metal Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 7282-7293.	1.5	20
45	Molybdenum disulfide for ultra-low detection of free radicals: electrochemical response and molecular modeling. 2D Materials, 2017, 4, 025077.	2.0	21
46	Adsorbate doping of MoS₂and WSe₂: the influence of Na and Co. Journal of Physics Condensed Matter, 2017, 29, 285501.	0.7	12
47	Diffusion of small Cu islands on the Ni(111) surface: A self-learning kinetic Monte Carlo study. Surface Science, 2017, 662, 42-58.	0.8	13
48	MoS₂-supported gold nanoparticle for CO hydrogenation. Journal of Physics Condensed Matter, 2017, 29, 415201.	0.7	12
49	Adatom Extraction from Pristine Metal Terraces by Dissociative Oxygen Adsorption: Combined STM and Density Functional Theory Investigation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">O</mml:mi><mml:mo>/</mml:mo><mml:mi>Ag</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 242 Td (stretchy="fals	2.9	11
50	Nonadiabatic exchange-correlation kernel for strongly correlated materials. Journal of Physics Condensed Matter, 2017, 29, 455601.	0.7	8
51	Time-Dependent Density-Functional Theory and Excitons in Bulk and Two-Dimensional Semiconductors. Computation, 2017, 5, 39.	1.0	19
52	Ptâ€“dipyridyl tetrazine metalâ€“organic network on the Au(100) surface: insights from first principles calculations. Faraday Discussions, 2017, 204, 83-95.	1.6	4
53	Towards TDDFT for Strongly Correlated Materials. Computation, 2016, 4, 34.	1.0	3
54	Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride. ACS Omega, 2016, 1, 1343-1354.	1.6	43

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55	pH-Induced Surface Modification of Atomically Precise Silver Nanoclusters: An Approach for Tunable Optical and Electronic Properties. Inorganic Chemistry, 2016, 55, 11522-11528.	1.9	10
56	Adsorption, diffusion, and vibration of oxygen on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ag</mml:mi><mml:mo>(</mml:mo><mml:mn>1 Physical Review B, 2015, 92, .	1.1	21
57	Effect of structure on the magnetic anisotropy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>L</mml:mi><mml:msub><mml:mn>1 nanoparticles. Physical Review B, 2015, 92, .	1.1	20
58	Geometric and electronic structure and magnetic properties of Feâ€“Au nanoalloys: insights from ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 28177-28185.	1.3	12
59	Friedel oscillations responsible for stacking fault of adatoms: The case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mrow><mml:mi>Mg</mml:mi><mml:mo>(</mml:mo> xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Be</mml:mi><mml:mo>(</mml:mo><mml:mn>0001 Physical Review B, 2015, 91, .	1.1	2
60	Revisiting the surface properties of Mg(0001) thin films and their effect on the adatom binding energy and self-diffusion. Surface Science, 2015, 632, 14-19.	0.8	3
61	Nonadiabatic time-dependent spin-density functional theory for strongly correlated systems. Journal of Physics Condensed Matter, 2014, 26, 022201.	0.7	12
62	Time-dependent density-matrix functional theory for trion excitations: Application to monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">MoS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>and other transition-metal dichalcogenides. Physical Review B, 2014, 90, .	1.1	26
63	Occupied and unoccupied electronic structure of Na doped MoS2(0001). Applied Physics Letters, 2014, 105, .	1.5	30
64	Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application. Journal of Physical Chemistry C, 2014, 118, 5346-5351.	1.5	260
65	Combined Density Functional Theory and Kinetic Monte Carlo Study of Selective Oxidation of NH₃ on Rutile RuO₂(110) at Ambient Pressures. Journal of Physical Chemistry C, 2014, 118, 5226-5238.	1.5	16
66	Anomalously Soft and Stiff Modes of Transition-Metal Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 10335-10347.	1.5	13
67	Joined edges in MoS₂: metallic and half-metallic wires. Journal of Physics Condensed Matter, 2013, 25, 312201.	0.7	21
68	Growth of aligned Mo6S6 nanowires on Cu(111). Surface Science, 2013, 611, 1-4.	0.8	20
69	Deactivation of Cu2O(100) by CO Poisoning. Topics in Catalysis, 2013, 56, 1082-1087.	1.3	4
70	Kinetically driven shape changes in early stages of two-dimensional island coarsening: Ag/Ag(111). Physical Review B, 2013, 88, .	1.1	5
71	Self-diffusion of small Ni clusters on the Ni(111) surface: A self-learning kinetic Monte Carlo study. Physical Review B, 2013, 88, .	1.1	14
72	Methanol Reaction on Ptâ€“Au Clusters on TiO₂(110): Methoxy-Induced Diffusion of Pt. Journal of Physical Chemistry C, 2013, 117, 26998-27006.	1.5	21

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73	Rationale for the Higher Reactivity of Interfacial Sites in Methanol Decomposition on Au₁₃/TiO₂(110). Journal of the American Chemical Society, 2013, 135, 7629-7635.	6.6	56
74	Controlled argon beam-induced desulfurization of monolayer molybdenum disulfide. Journal of Physics Condensed Matter, 2013, 25, 252201.	0.7	75
75	Vibrations of Au₁₃and FeAu₁₂nanoparticles and the limits of the Debye temperature concept. Journal of Physics Condensed Matter, 2012, 24, 104026.	0.7	16
76	Optical Generation of Collective Plasmon Modes in Small Gold Chains Induced by Doping Transition-Metal Impurities. Physical Review Letters, 2012, 109, 157404.	2.9	26
77	Extended pattern recognition scheme for self-learning kinetic Monte Carlo simulations. Journal of Physics Condensed Matter, 2012, 24, 354004.	0.7	5
78	Tailoring Electronic Structure Through Alloying: The AgnCu34â€“n(n= 0â€“34) Nanoparticle Family. Journal of Physical Chemistry C, 2012, 116, 281-291.	1.5	31
79	The Quantum Magnetism of Individual Manganese-12-Acetate Molecular Magnets Anchored at Surfaces. Nano Letters, 2012, 12, 518-521.	4.5	146
80	An MoS_x Structure with High Affinity for Adsorbate Interaction. Angewandte Chemie - International Edition, 2012, 51, 10284-10288.	7.2	13
81	Single layer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>on the Cu(111) surface: First-principles electronic structure calculations. Physical Review B, 2012, 85, .	1.1	26
82	Dissociative Hydrogen Adsorption on Close-Packed Cobalt Nanoparticle Surfaces. Journal of Physical Chemistry C, 2012, 116, 25868-25873.	1.5	35
83	Off-lattice pattern recognition scheme for kinetic Monte Carlo simulations. Journal of Computational Physics, 2012, 231, 3548-3560.	1.9	17
84	CO-Induced Diffusion of Ni Atoms to the Surface of Niâ€“Au Clusters on TiO₂(110). Journal of Physical Chemistry C, 2011, 115, 11112-11123.	1.5	60
85	Toward an Understanding of Ligand Selectivity in Nanocluster Synthesis. Journal of Physical Chemistry C, 2011, 115, 14478-14487.	1.5	28
86	The crossover from collective motion to periphery diffusion for two-dimensional adatom-islands on Cu(111). Journal of Physics Condensed Matter, 2011, 23, 462201.	0.7	12
87	Vibrations at surfaces. Journal of Physics Condensed Matter, 2011, 23, 480301.	0.7	0
88	Island-size selectivity during 2D Ag island coarsening on Ag(111). Journal of Physics Condensed Matter, 2011, 23, 262001.	0.7	4
89	Toward the Growth of an Aligned Single-Layer MoS₂ Film. Langmuir, 2011, 27, 11650-11653.	1.6	84
90	Effect of misfit dislocation on surface diffusion. Physical Review B, 2011, 84, .	1.1	8

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91	Diffusion of the Cu monomer and dimer on Ag(111): Molecular dynamics simulations and density functional theory calculations. Physical Review B, 2010, 82, .	1.1	28
92	Surface vibrational thermodynamics from ab initio calculations for fcc(100). Surface Science, 2010, 604, 308-317.	0.8	5
93	Selective oxidation of ammonia on RuO2(110): A combined DFT and KMC study. Journal of Catalysis, 2010, 276, 371-381.	3.1	52
94	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. Physical Review B, 2010, 82, .	1.1	18
95	Vibrational dynamics of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mo induced by nitrogen adsorption on Cu(001). Physical Review B, 2010, 81, .	1.1	4
96	Time-dependent density-matrix functional theory for biexcitonic phenomena. Physical Review B, 2010, 82, .	1.1	4
97	Comparative study of CO adsorption on flat, stepped, and kinked Au surfaces using density functional theory. Physical Review B, 2009, 79, .	1.1	50
98	Off-lattice self-learning kinetic Monte Carlo: application to 2D cluster diffusion on the fcc(111) surface. Journal of Physics Condensed Matter, 2009, 21, 084213.	0.7	37
99	Parallel kinetic Monte Carlo simulations of Ag(111) island coarsening using a large database. Journal of Physics Condensed Matter, 2009, 21, 084214.	0.7	21
100	Reactivity of the Cu2O(1 0 0) surface: Insights from first principles calculations. Surface Science, 2009, 603, 1637-1645.	0.8	70
101	Effect of Ligands on the Geometric and Electronic Structure of Au13 Clusters. Journal of Physical Chemistry C, 2009, 113, 12072-12078.	1.5	99
102	Structural, vibrational and thermodynamic properties of Ag_nCu_{34â˜n}nanoparticles. Journal of Physics Condensed Matter, 2009, 21, 084220.	0.7	13
103	Origin of quasi-constant pre-exponential factors for adatom diffusion on Cu and Ag surfaces. Physical Review B, 2007, 76, .	1.1	24
104	Diffusion of small two-dimensional Cu islands on Cu(111) studied with a kinetic Monte Carlo method. Physical Review B, 2006, 73, .	1.1	58
105	Complete CO Oxidation over Cu2O Nanoparticles Supported on Silica Gel. Nano Letters, 2006, 6, 2095-2098.	4.5	265
106	Calculated pre-exponential factors and energetics for adatom hopping on terraces and steps of Cu(100) and Cu(110). Surface Science, 2006, 600, 484-492.	0.8	43
107	Effect of step-step separation on surface diffusion processes. Physical Review B, 2006, 73, .	1.1	18
108	Energetics ofCOon stepped and kinked Cu surfaces: A comparative theoretical study. Physical Review B, 2006, 74, .	1.1	29

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109	Vibrational dynamics and thermodynamics of surfaces and nanostructures. Surface Science Reports, 2005, 56, 159-187.	3.8	54
110	Self-learning kinetic Monte Carlo method: Application to Cu(111). Physical Review B, 2005, 72, .	1.1	114
111	Site selectivity in chemisorption of C on Pd(211). Physical Review B, 2004, 70, .	1.1	16
112	Cluster Diffusion and Coalescence on Metal Surfaces: applications of a Self-learning Kinetic Monte-Carlo method. Materials Research Society Symposia Proceedings, 2004, 859, 1.	0.1	1
113	Vibrational Dynamics and Excess Entropy of Multi-grain Nanoparticles. Journal of Computational and Theoretical Nanoscience, 2004, 1, 216-220.	0.4	9
114	Local and excess vibrational free energies of stepped metal surfaces. Physical Review B, 2003, 67, .	1.1	24
115	Structure of Ag(410) and Cu(320). Physical Review B, 2003, 67, .	1.1	22
116	Structural relaxations, vibrational dynamics and thermodynamics of vicinal surfaces. Journal of Physics Condensed Matter, 2003, 15, S3197-S3226.	0.7	27
117	Comparative study of anharmonicity: Ni(111), Cu(111), and Ag(111). Physical Review B, 2002, 66, .	1.1	20
118	Electronic structure of thec(2Ã—2)O/Cu(001)system. Physical Review B, 2002, 66, .	1.1	20
119	Ab initiocalculations of multilayer relaxations of stepped Cu surfaces. Physical Review B, 2002, 65, .	1.1	36
120	Relationship between electronic and geometric structures of the O/Cu(001) system. Journal of Chemical Physics, 2002, 117, 8523-8530.	1.2	15
121	Anharmonic effects on Ag(111): a molecular dynamics study. Surface Science, 2000, 446, 17-30.	0.8	32
122	Multilayer relaxations and stresses on Mg surfaces. Physical Review B, 1999, 60, 15613-15616.	1.1	26
123	Vibrational Properties of Metallic Nanocrystals. Physical Review Letters, 1998, 81, 1453-1456.	2.9	169
124	Vibrational dynamics and thermodynamics of Ni(977). Journal of Chemical Physics, 1997, 106, 2031-2037.	1.2	36
125	Local structural and vibrational properties of stepped surfaces: Cu(211), Cu(511), and Cu(331). Physical Review B, 1997, 55, 13894-13903.	1.1	60
126	Diffusion Processes and Pre-Exponential Factors in Homo-Epitaxial Growth on Ag(100). Materials Research Society Symposia Proceedings, 1997, 492, 263.	0.1	0

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127	Vibrational free energy contribution to self-diffusion on Ni(100), Cu(100) and Ag(100). Surface Science, 1997, 383, 137-148.	0.8	31
128	Role of Lattice Vibrations in Adatom Diffusion. Physical Review Letters, 1997, 78, 1086-1089.	2.9	94
129	Local thermodynamic properties of a stepped metal surface: Cu(711). Physical Review B, 1996, 53, 15489-15492.	1.1	35
130	Surface vibrations of Ag(100) and Cu(100): A molecular-dynamics study. Physical Review B, 1991, 44, 13725-13733.	1.1	72
131	Enhanced anharmonicity on Cu(110). Physical Review Letters, 1991, 67, 2327-2330.	2.9	105
132	On the dynamics of the associative desorption of H2. Journal of Chemical Physics, 1988, 89, 4427-4439.	1.2	99
133	Electron energy loss spectroscopy of adsorbed atoms. Journal of Vacuum Science and Technology, 1982, 20, 567-573.	1.9	9