Talat S Rahman

List of Publications by Year
in descending order

133 papers	3,697 citations	159585 30 h-index	155660 55 g-index
136 all docs	136 docs citations	136 times ranked	4549 citing authors

#	Article	IF	Citations
1	Complete CO Oxidation over Cu2O Nanoparticles Supported on Silica Gel. Nano Letters, 2006, 6, 2095-2098.	9.1	265
2	Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application. Journal of Physical Chemistry C, 2014, 118, 5346-5351.	3.1	260
3	Vibrational Properties of Metallic Nanocrystals. Physical Review Letters, 1998, 81, 1453-1456.	7.8	169
4	The Quantum Magnetism of Individual Manganese-12-Acetate Molecular Magnets Anchored at Surfaces. Nano Letters, 2012, 12, 518-521.	9.1	146
5	Self-learning kinetic Monte Carlo method: Application to Cu(111). Physical Review B, 2005, 72, .	3.2	114
6	Enhanced anharmonicity on Cu(110). Physical Review Letters, 1991, 67, 2327-2330.	7.8	105
7	On the dynamics of the associative desorption of H2. Journal of Chemical Physics, 1988, 89, 4427-4439.	3.0	99
8	Effect of Ligands on the Geometric and Electronic Structure of Au13 Clusters. Journal of Physical Chemistry C, 2009, 113, 12072-12078.	3.1	99
9	Role of Lattice Vibrations in Adatom Diffusion. Physical Review Letters, 1997, 78, 1086-1089.	7.8	94
10	Toward the Growth of an Aligned Single-Layer MoS₂ Film. Langmuir, 2011, 27, 11650-11653.	3.5	84
11	Controlled argon beam-induced desulfurization of monolayer molybdenum disulfide. Journal of Physics Condensed Matter, 2013, 25, 252201.	1.8	75
12	Surface vibrations of Ag(100) and Cu(100): A molecular-dynamics study. Physical Review B, 1991, 44, 13725-13733.	3.2	72
13	Reactivity of the Cu2O(1 0 0) surface: Insights from first principles calculations. Surface Science, 2009, 603, 1637-1645.	1.9	70
14	Local structural and vibrational properties of stepped surfaces: Cu(211), Cu(511), and Cu(331). Physical Review B, 1997, 55, 13894-13903.	3.2	60
15	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.	3.1	60
16	Diffusion of small two-dimensional Cu islands on Cu(111) studied with a kinetic Monte Carlo method. Physical Review B, 2006, 73, .	3.2	58
17	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.	13.7	56
18	Vibrational dynamics and thermodynamics of surfaces and nanostructures. Surface Science Reports, 2005, 56, 159-187.	7.2	54

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19	Selective oxidation of ammonia on RuO2(110): A combined DFT and KMC study. Journal of Catalysis, 2010, 276, 371-381.	6.2	52
20	Comparative study of CO adsorption on flat, stepped, and kinked Au surfaces using density functional theory. Physical Review B, 2009, 79, .	3.2	50
21	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.	1.9	43
22	Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride. ACS Omega, 2016, 1, 1343-1354.	3.5	43
23	CO Oxidation Mechanisms on CoO_x-Pt Thin Films. Journal of the American Chemical Society, 2020, 142, 8312-8322.	13.7	39
24	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.	1.8	37
25	Vibrational dynamics and thermodynamics of Ni(977). Journal of Chemical Physics, 1997, 106, 2031-2037.	3.0	36
26	Ab initiocalculations of multilayer relaxations of stepped Cu surfaces. Physical Review B, 2002, 65, .	3.2	36
27	Local thermodynamic properties of a stepped metal surface: Cu(711). Physical Review B, 1996, 53, 15489-15492.	3.2	35
28	Dissociative Hydrogen Adsorption on Close-Packed Cobalt Nanoparticle Surfaces. Journal of Physical Chemistry C, 2012, 116, 25868-25873.	3.1	35
29	Ultrafast Electron Correlations and Memory Effects at Work: Femtosecond Demagnetization in Ni. Physical Review Letters, 2020, 125, 017202.	7.8	35
30	Anharmonic effects on Ag(111): a molecular dynamics study. Surface Science, 2000, 446, 17-30.	1.9	32
31	Vibrational free energy contribution to self-diffusion on Ni(100), Cu(100) and Ag(100). Surface Science, 1997, 383, 137-148.	1.9	31
32	Tailoring Electronic Structure Through Alloying: The AgnCu34â€“n(n= 0â€“34) Nanoparticle Family. Journal of Physical Chemistry C, 2012, 116, 281-291.	3.1	31
33	Occupied and unoccupied electronic structure of Na doped MoS2(0001). Applied Physics Letters, 2014, 105, .	3.3	30
34	Energetics ofCOon stepped and kinked Cu surfaces: A comparative theoretical study. Physical Review B, 2006, 74, .	3.2	29
35	Diffusion of the Cu monomer and dimer on Ag(111): Molecular dynamics simulations and density functional theory calculations. Physical Review B, 2010, 82, .	3.2	28
36	Toward an Understanding of Ligand Selectivity in Nanocluster Synthesis. Journal of Physical Chemistry C, 2011, 115, 14478-14487.	3.1	28

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37	Structural relaxations, vibrational dynamics and thermodynamics of vicinal surfaces. Journal of Physics Condensed Matter, 2003, 15, S3197-S3226.	1.8	27
38	Multilayer relaxations and stresses on Mg surfaces. Physical Review B, 1999, 60, 15613-15616.	3.2	26
39	Optical Generation of Collective Plasmon Modes in Small Gold Chains Induced by Doping Transition-Metal Impurities. Physical Review Letters, 2012, 109, 157404.	7.8	26
40	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, .	3.2	26
41	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, .	3.2	26
42	Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride. ACS Sustainable Chemistry and Engineering, 2021, 9, 2447-2455.	6.7	25
43	Local and excess vibrational free energies of stepped metal surfaces. Physical Review B, 2003, 67, .	3.2	24
44	Origin of quasi-constant pre-exponential factors for adatom diffusion on Cu and Ag surfaces. Physical Review B, 2007, 76, .	3.2	24
45	Redox-active ligand controlled selectivity of vanadium oxidation on Au(100). Chemical Science, 2018, 9, 1674-1685.	7.4	24
46	Structure of Ag(410) and Cu(320). Physical Review B, 2003, 67, .	3.2	22
47	Parallel kinetic Monte Carlo simulations of Ag(111) island coarsening using a large database. Journal of Physics Condensed Matter, 2009, 21, 084214.	1.8	21
48	Joined edges in MoS₂: metallic and half-metallic wires. Journal of Physics Condensed Matter, 2013, 25, 312201.	1.8	21
49	Methanol Reaction on Ptâ€“Au Clusters on TiO₂(110): Methoxy-Induced Diffusion of Pt. Journal of Physical Chemistry C, 2013, 117, 26998-27006.	3.1	21
50	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>110</mml:mn></mml:mrow></mml:math>: Physical Review B, 2015, 92, .	3.2	21
51	Molybdenum disulfide for ultra-low detection of free radicals: electrochemical response and molecular modeling. 2D Materials, 2017, 4, 025077.	4.4	21
52	Plasmon Excitations in Mixed Metallic Nanoarrays. ACS Nano, 2019, 13, 5344-5355.	14.6	21
53	Electron thermalization and relaxation in laser-heated nickel by few-femtosecond core-level transient absorption spectroscopy. Physical Review B, 2021, 103, .	3.2	21
54	Comparative study of anharmonicity: Ni(111), Cu(111), and Ag(111). Physical Review B, 2002, 66, .	3.2	20

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55	Electronic structure of thec(2Ã—2)O/Cu(001)system. Physical Review B, 2002, 66, .	3.2	20
56	Growth of aligned Mo6S6 nanowires on Cu(111). Surface Science, 2013, 611, 1-4.	1.9	20
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</mml:mn> nanoparticles. Physical Review B, 2015, 92, .	3.2	20
58	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.	3.1	20
59	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.	6.7	20
60	Time-Dependent Density-Functional Theory and Excitons in Bulk and Two-Dimensional Semiconductors. Computation, 2017, 5, 39.	2.0	19
61	Effect of step-step separation on surface diffusion processes. Physical Review B, 2006, 73, .	3.2	18
62	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. Physical Review B, 2010, 82, .	3.2	18
63	MoS₂ Nanoclusters Grown on TiO₂: Evidence for New Adsorption Sites at Edges and Sulfur Vacancies. Journal of Physical Chemistry C, 2019, 123, 7185-7201.	3.1	18
64	Off-lattice pattern recognition scheme for kinetic Monte Carlo simulations. Journal of Computational Physics, 2012, 231, 3548-3560.	3.8	17
65	Metallicity of 2H-MoS₂ induced by Au hybridization. 2D Materials, 2020, 7, 025021.	4.4	17
66	Site selectivity in chemisorption of C on Pd(211). Physical Review B, 2004, 70, .	3.2	16
67	Vibrations of Au₁₃and FeAu₁₂nanoparticles and the limits of the Debye temperature concept. Journal of Physics Condensed Matter, 2012, 24, 104026.	1.8	16
68	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.	3.1	16
69	Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS₂. Journal of Physical Chemistry C, 2018, 122, 267-273.	3.1	16
70	Asymmetric Design of Spin-Crossover Complexes to Increase the Volatility for Surface Deposition. Journal of the American Chemical Society, 2021, 143, 14563-14572.	13.7	16
71	Relationship between electronic and geometric structures of the O/Cu(001) system. Journal of Chemical Physics, 2002, 117, 8523-8530.	3.0	15
72	Self-diffusion of small Ni clusters on the Ni(111) surface: A self-learning kinetic Monte Carlo study. Physical Review B, 2013, 88, .	3.2	14

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73	Structural, vibrational and thermodynamic properties of Ag_nCu_{34â"n}nanoparticles. Journal of Physics Condensed Matter, 2009, 21, 084220.	1.8	13
74	An MoS_x Structure with High Affinity for Adsorbate Interaction. Angewandte Chemie - International Edition, 2012, 51, 10284-10288.	13.8	13
75	Anomalously Soft and Stiff Modes of Transition-Metal Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 10335-10347.	3.1	13
76	Diffusion of small Cu islands on the Ni(111) surface: A self-learning kinetic Monte Carlo study. Surface Science, 2017, 662, 42-58.	1.9	13
77	The crossover from collective motion to periphery diffusion for two-dimensional adatom-islands on Cu(111). Journal of Physics Condensed Matter, 2011, 23, 462201.	1.8	12
78	Nonadiabatic time-dependent spin-density functional theory for strongly correlated systems. Journal of Physics Condensed Matter, 2014, 26, 022201.	1.8	12
79	Geometric and electronic structure and magnetic properties of Feâ€"Au nanoalloys: insights from ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 28177-28185.	2.8	12
80	Adsorbate doping of MoS₂and WSe₂: the influence of Na and Co. Journal of Physics Condensed Matter, 2017, 29, 285501.	1.8	12
81	MoS₂-supported gold nanoparticle for CO hydrogenation. Journal of Physics Condensed Matter, 2017, 29, 415201.	1.8	12
82	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 362 Td (stretchy="false">)</mm	7.8	11
83	Methoxy Formation Induced Defects on MoS₂. Journal of Physical Chemistry C, 2018, 122, 10042-10049.	3.1	11
84	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.	3.1	11
85	Characteristics of Single-Molecule Magnet Dimers ([Mn₃]₂) on Graphene and h-BN. Journal of Physical Chemistry C, 2020, 124, 28186-28200.	3.1	11
86	Plasmon excitations in chemically heterogeneous nanoarrays. Physical Review B, 2020, 101, .	3.2	11
87	Anisotropic Properties of Quasiâ€1D In₄Se₃: Mechanical Exfoliation, Electronic Transport, and Polarizationâ€Dependent Photoresponse. Advanced Functional Materials, 2021, 31, 2106459.	14.9	11
88	pH-Induced Surface Modification of Atomically Precise Silver Nanoclusters: An Approach for Tunable Optical and Electronic Properties. Inorganic Chemistry, 2016, 55, 11522-11528.	4.0	10
89	Atomic-Scale Structure and Catalysis on Positively Charged Bimetallic Sites for Generation of H₂. Nano Letters, 2020, 20, 6255-6262.	9.1	10
90	Electron energy loss spectroscopy of adsorbed atoms. Journal of Vacuum Science and Technology, 1982, 20, 567-573.	1.9	9

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91	Syngas molecules as probes for defects in 2D hexagonal boron nitride: their adsorption and vibrations. Physical Chemistry Chemical Physics, 2021, 23, 7988-8001.	2.8	9
92	Vibrational Dynamics and Excess Entropy of Multi-grain Nanoparticles. Journal of Computational and Theoretical Nanoscience, 2004, 1, 216-220.	0.4	9
93	Effect of misfit dislocation on surface diffusion. Physical Review B, 2011, 84, .	3.2	8
94	Nonadiabatic exchange-correlation kernel for strongly correlated materials. Journal of Physics Condensed Matter, 2017, 29, 455601.	1.8	8
95	Ligand-coordination effects on the selective hydrogenation of acetylene in single-site Pd-ligand supported catalysts. Journal of Catalysis, 2022, 413, 81-92.	6.2	8
96	Redox Isomeric Surface Structures Are Preferred over Oddâ€Electron Pt 1+. Chemistry - A European Journal, 2018, 24, 15852-15858.	3.3	7
97	Effects of Î³-Al2O3 Support on the Morphology and Electronic Structure of Pt Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 16893-16901.	3.1	7
98	Multiâ€electron Reduction Capacity and Multiple Binding Pockets in Metalâ€“Organic Redox Assembly at Surfaces. Chemistry - A European Journal, 2019, 25, 5565-5573.	3.3	7
99	Ultrafast charge dynamics and photoluminescence in bilayer MoS₂. 2D Materials, 2021, 8, 025018.	4.4	7
100	Deciphering complex features in STM images of O adatoms on Ag(110). Physical Review B, 2018, 98, .	3.2	6
101	Anisotropy-exchange resonance as a mechanism for entangled state switching. Physical Review A, 2021, 104, .	2.5	6
102	Surface vibrational thermodynamics from ab initio calculations for fcc(100). Surface Science, 2010, 604, 308-317.	1.9	5
103	Extended pattern recognition scheme for self-learning kinetic Monte Carlo simulations. Journal of Physics Condensed Matter, 2012, 24, 354004.	1.8	5
104	Kinetically driven shape changes in early stages of two-dimensional island coarsening: Ag/Ag(111). Physical Review B, 2013, 88, .	3.2	5
105	Toward multiscale modeling of thin-film growth processes using SLKMC. Journal of Materials Research, 2018, 33, 709-719.	2.6	5
106	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.	1.1	5
107	Growth of Graphene Nanoflakes/hâ€BN Heterostructures. Advanced Materials Interfaces, 2021, 8, 2100766.	3.7	5
108	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>2×2</mml:mn><mml:mo> induced by nitrogen adsorption on Cu(001). Physical Review B, 2010, 81, .	3.2	4

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109	Time-dependent density-matrix functional theory for biexcitonic phenomena. Physical Review B, 2010, 82, .	3.2	4
110	Island-size selectivity during 2D Ag island coarsening on Ag(111). Journal of Physics Condensed Matter, 2011, 23, 262001.	1.8	4
111	Deactivation of Cu2O(100) by CO Poisoning. Topics in Catalysis, 2013, 56, 1082-1087.	2.8	4
112	Fermi surfaces of the topological semimetal CaSn₃ probed through de Haas van Alphen oscillations. Journal of Physics Condensed Matter, 2021, 33, 17LT01.	1.8	4
113	Ptâ€“dipyridyl tetrazine metalâ€“organic network on the Au(100) surface: insights from first principles calculations. Faraday Discussions, 2017, 204, 83-95.	3.2	4
114	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.	1.9	3
115	Towards TDDFT for Strongly Correlated Materials. Computation, 2016, 4, 34.	2.0	3
116	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.	3.0	3
117	Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS2 â€“ predictions from DFT+KMC. Journal of Chemical Physics, 2021, 154, 174701.	3.0	3
118	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></mml: xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Be</mml:mi><mml:mo>(</mml:mo><mml:mn>0001</mml:mn> Physical Review B, 2015, 91, .	3.2	2
119	Surface Thermodynamics and Vibrational Entropy. Springer Handbooks, 2020, , 71-93.	0.6	2
120	Defect engineering of oxide surfaces: dream or reality?. Journal of Physics Condensed Matter, 2022, 34, 291501.	1.8	2
121	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
122	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. Physical Review B, 2021, 103, .	3.2	1
123	On stabilizing spin crossover molecule [Fe(tBu₂qsal)₂] on suitable supports: insights from ab initio studies. Journal of Physics Condensed Matter, 2021, 33, 385201.	1.8	1
124	Tailoring the redox capabilities of organic ligands for metal-ligand coordination with vanadium single-sites. Surface Science, 2021, 712, 121888.	1.9	1
125	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.	1.8	1
126	Methanol carbonylation to acetaldehyde on Au particles supported by single-layer MoS₂ grown on silica. Journal of Physics Condensed Matter, 2022, 34, 104005.	1.8	1

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127	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.	4.6	1
128	Diffusion Processes and Pre-Exponential Factors in Homo-Epitaxial Growth on Ag(100). Materials Research Society Symposia Proceedings, 1997, 492, 263.	0.1	0
129	Vibrations at surfaces. Journal of Physics Condensed Matter, 2011, 23, 480301.	1.8	0
130	MoS2-supported Au31 for CO hydrogenation: A first-principle study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, 032201.	2.1	0
131	Excited states in hydrogenated single-layer MoS₂. Journal of Physics Condensed Matter, 2021, 33, 075201.	1.8	0
132	Atomic and molecular functionalisation of technological materials: an introduction to nanoscale processes on semiconductor surfaces. Journal of Physics Condensed Matter, 2022, 34, 210401.	1.8	0
133	Nonadiabatic Exchange-Correlation Potential for Strongly Correlated Materials in the Weak and Strong Interaction Limits. Computation, 2022, 10, 77.	2.0	0