Mal Soon Lee

List of Publications by Year
in descending order

63 papers	2,343 citations	201658 27 h-index	214788 47 g-index
70 all docs	70 docs citations	70 times ranked	3066 citing authors

#	Article	IF	Citations
1	Electrocatalytic Hydrogenation of Biomass-Derived Organics: A Review. Chemical Reviews, 2020, 120, 11370-11419.	47.7	185
2	CO Oxidation on Au/TiO₂: Condition-Dependent Active Sites and Mechanistic Pathways. Journal of the American Chemical Society, 2016, 138, 10467-10476.	13.7	159
3	Genesis and Stability of Hydronium Ions in Zeolite Channels. Journal of the American Chemical Society, 2019, 141, 3444-3455.	13.7	119
4	Electronic structure and thermoelectric properties of Sb-based semiconducting half-Heusler compounds. Physical Review B, 2011, 83, .	3.2	106
5	High-pressure polymeric phases of carbon dioxide. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6077-6081.	7.1	104
6	Competitive sorption of CO2 and H2O in 2:1 layer phyllosilicates. Geochimica Et Cosmochimica Acta, 2015, 161, 248-257.	3.9	98
7	Impeding 99Tc(IV) mobility in novel waste forms. Nature Communications, 2016, 7, 12067.	12.8	94
8	Validity of the rigid band approximation in the study of the thermopower of narrow band gap semiconductors. Physical Review B, 2012, 85, .	3.2	93
9	Understanding the Role of Metal and Molecular Structure on the Electrocatalytic Hydrogenation of Oxygenated Organic Compounds. ACS Catalysis, 2019, 9, 9964-9972.	11.2	81
10	Anharmonicity and Confinement in Zeolites: Structure, Spectroscopy, and Adsorption Free Energy of Ethanol in H-ZSM-5. Journal of Physical Chemistry C, 2016, 120, 7172-7182.	3.1	77
11	A Combined Experimental and Theoretical Study on the Activity and Selectivity of the Electrocatalytic Hydrogenation of Aldehydes. ACS Catalysis, 2018, 8, 7645-7658.	11.2	76
12	Effect of Collective Dynamics and Anharmonicity on Entropy in Heterogenous Catalysis: Building the Case for Advanced Molecular Simulations. ACS Catalysis, 2020, 10, 9236-9260.	11.2	63
13	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie - International Edition, 2019, 58, 3527-3532.	13.8	62
14	Impact of pH on Aqueous-Phase Phenol Hydrogenation Catalyzed by Carbon-Supported Pt and Rh. ACS Catalysis, 2019, 9, 1120-1128.	11.2	55
15	Environment of Metalâ€“Oâ€“Fe Bonds Enabling High Activity in CO₂ Reduction on Single Metal Atoms and on Supported Nanoparticles. Journal of the American Chemical Society, 2021, 143, 5540-5549.	13.7	54
16	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 1501-1505.	13.8	53
17	Effect of onsite Coulomb repulsion on thermoelectric properties of full-Heusler compounds with pseudogaps. Physical Review B, 2011, 84, .	3.2	52
18	Microstructural Response of Variably Hydrated Ca-rich Montmorillonite to Supercritical CO₂. Environmental Science & Technology, 2014, 48, 8612-8619.	10.0	52

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19	First-principles investigation of finite-temperature behavior in small sodium clusters. Journal of Chemical Physics, 2005, 123, 164310.	3.0	51
20	Structural Rearrangement of Auâ€“Pd Nanoparticles under Reaction Conditions: An ab Initio Molecular Dynamics Study. ACS Nano, 2017, 11, 1649-1658.	14.6	47
21	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	13.8	40
22	Far-infrared absorption of water clusters by first-principles molecular dynamics. Journal of Chemical Physics, 2008, 128, 214506.	3.0	39
23	Aluminum Zintl anion moieties within sodium aluminum clusters. Journal of Chemical Physics, 2014, 140, 054301.	3.0	37
24	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie - International Edition, 2021, 60, 22769-22775.	13.8	34
25	Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. Journal of Physical Chemistry Letters, 2016, 7, 1646-1652.	4.6	33
26	Finite-Temperature Effects on the Stability and Infrared Spectra of HCl(H₂O)₆ Clusters. Journal of Physical Chemistry A, 2007, 111, 12810-12815.	2.5	31
27	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	4.1	29
28	Thermodynamic stability of layered structures in compressed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2009, 79, .	3.2	26
29	Structure, dynamics and stability of water/scCO2/mineral interfaces from ab initio molecular dynamics simulations. Scientific Reports, 2015, 5, 14857.	3.3	26
30	Molecular Level Investigation of CH₄ and CO₂ Adsorption in Hydrated Calciumâ€“Montmorillonite. Journal of Physical Chemistry C, 2018, 122, 1125-1134.	3.1	26
31	Mixtures of planetary ices at extreme conditions. Nature Communications, 2011, 2, 185.	12.8	22
32	Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts. Journal of Catalysis, 2020, 386, 30-38.	6.2	22
33	Activity of Cuâ€“Alâ€“Oxo Extra-Framework Clusters for Selective Methane Oxidation on Cu-Exchanged Zeolites. Jacs Au, 2021, 1, 1412-1421.	7.9	21
34	The effects of electronic structure and charged state on thermodynamic properties: An ab initio molecular dynamics investigations on neutral and charged clusters of Na39, Na40, and Na41. Journal of Chemical Physics, 2008, 128, 104701.	3.0	19
35	Physics of bandgap formation in Cuâ€“Sbâ€“Se based novel thermoelectrics: the role of Sb valency and Cu d levels. Journal of Physics Condensed Matter, 2012, 24, 415502.	1.8	19
36	Electrochemically Tunable Protonâ€Coupled Electron Transfer in Pdâ€Catalyzed Benzaldehyde Hydrogenation. Angewandte Chemie, 2020, 132, 1517-1521.	2.0	18

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37	Effects of geometric and electronic structure on the finite temperature behavior ofNa58,Na57, andNa55cluster. Physical Review B, 2007, 75, .	3.2	17
38	Diffusion and Surface Segregation of Interstitial Ti Defects Induced by Electronic Metalâ€“Support Interactions on a Au/TiO₂ Nanocatalyst. ACS Catalysis, 2022, 12, 4455-4464.	11.2	17
39	SixC1âˆ’xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
40	Controlling Metalâ€“Organic Framework/ZnO Heterostructure Kinetics through Selective Ligand Binding to ZnO Surface Steps. Chemistry of Materials, 2020, 32, 6666-6675.	6.7	16
41	Geometry, electronic properties, and thermodynamics of pure and Al-doped Li clusters. Physical Review B, 2006, 74, .	3.2	15
42	Electronic structures, equilibrium geometries, and finite-temperature properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">Na</mml:mi><mml:mi>n</mml:mi></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>(</mml:mo><mml:mi>n</mml:mi><mml:mo>=</mml:mo><mml:mn>39</mml:mn><mml:mo>â	3.2	14
43	first principles. Physical Review B, 2007, 76, . Electro-reduction of organics on metal cathodes: A multiscale-modeling study of benzaldehyde on Au (111). Catalysis Today, 2020, 350, 39-46.	4.4	13
44	First-principle investigation on catalytic hydrogenation of benzaldehyde over Pt-group metals. Catalysis Today, 2022, 388-389, 208-215.	4.4	12
45	Selective acetylene hydrogenation over single metal atoms supported on Fe3O4(001): A first-principle study. Journal of Chemical Physics, 2020, 152, 154703.	3.0	12
46	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	2.0	12
47	Publisherâ€™s Note: Electronic structure and thermoelectric properties of Sb-based semiconducting half-Heusler compounds [Phys. Rev. B83, 085204 (2011)]. Physical Review B, 2011, 83, .	3.2	10
48	Interplay of topological surface and bulk electronic states in Bi<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>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	3.2	10
49	Creating self-assembled arrays of mono-oxo (MoO ₃) ₁ species on TiO ₂ (101) via deposition and decomposition of (MoO ₃) _n oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
50	Ab initiodensity-functional study of the equilibrium geometries and the electronic properties ofLi10âˆ’nSnn(n=0â€“10)clusters. Physical Review A, 2005, 72, .	2.5	9
51	Mechanistic Understanding of Catalytic Conversion of Ethanol to 1-Butene over 2D-Pillared MFI Zeolite. Journal of Physical Chemistry C, 2020, 124, 28437-28447.	3.1	9
52	Impact of functional groups on the electrocatalytic hydrogenation of aromatic carbonyls to alcohols. Catalysis Today, 2022, 397-399, 63-68.	4.4	5
53	Clusters. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 37-70.	0.6	3
54	Impact of Cr and Co on 99Tc retention in magnetite: A combined study of ab initio molecular dynamics and experiments. Journal of Hazardous Materials, 2020, 387, 121721.	12.4	3

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55	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	2.8	3
56	Binding and stability of MgO monomers on anatase TiO2(101). Journal of Chemical Physics, 2021, 154, 204703.	3.0	3
57	Molecular Simulation of the Catalytic Regeneration of ⁿBuLi through a Hydrometalation Route. Inorganic Chemistry, 2019, 58, 3033-3040.	4.0	2
58	The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie, 2019, 131, 3565-3570.	2.0	2
59	Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	3.5	2
60	Single-Atom Catalysis: An Analogy between Heterogeneous and Homogeneous Catalysts. ACS Symposium Series, 2020, , 1-15.	0.5	1
61	Berichtigung: The Nature of Hydrogen Adsorption on Platinum in the Aqueous Phase. Angewandte Chemie, 2020, 132, 13249-13249.	2.0	0
62	Defect-induced anisotropic surface reactivity and ion transfer processes of anatase nanoparticles. Materials Today Chemistry, 2020, 17, 100290.	3.5	0
63	Surface Density Dependent Catalytic Activity of Single Palladium Atoms Supported on Ceria**. Angewandte Chemie, 2021, 133, 22951.	2.0	0