Aravind Asthagiri

List of Publications by Year
in descending order

90 papers	5,216 citations	101543 36 h-index	88630 70 g-index
97 all docs	97 docs citations	97 times ranked	5742 citing authors

#	Article	IF	Citations
1	Selectivity of CO₂ Reduction on Copper Electrodes: The Role of the Kinetics of Elementary Steps. Angewandte Chemie - International Edition, 2013, 52, 2459-2462.	13.8	769
2	Facet Dependence of CO₂ Reduction Paths on Cu Electrodes. ACS Catalysis, 2016, 6, 219-229.	11.2	420
3	Reaction mechanisms of CO2 electrochemical reduction on Cu(111) determined with density functional theory. Journal of Catalysis, 2014, 312, 108-122.	6.2	382
4	Low-temperature activation of methane on the IrO ₂ (110) surface. Science, 2017, 356, 299-303.	12.6	244
5	Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents. Journal of Physical Chemistry B, 2001, 105, 4771-4782.	2.6	203
6	Dimeric [Mo₂S₁₂]^{2â^'} Cluster: A Molecular Analogue of MoS₂ Edges for Superior Hydrogenâ€Evolution Electrocatalysis. Angewandte Chemie - International Edition, 2015, 54, 15181-15185.	13.8	160
7	Alkane activation on crystalline metal oxide surfaces. Chemical Society Reviews, 2014, 43, 7536-7547.	38.1	133
8	Atomic-level simulation of ferroelectricity in oxide materials. Current Opinion in Solid State and Materials Science, 2005, 9, 107-113.	11.5	109
9	Solvation effects on DFT predictions of ORR activity on metal surfaces. Catalysis Today, 2019, 323, 35-43.	4.4	109
10	Density functional theory study of the initial oxidation of the Pt(111) surface. Physical Review B, 2009, 79, .	3.2	96
11	Second-generation charge-optimized many-body potential for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext> amorphous silica. Physical Review B, 2010, 82, .	3.2	90
12	First principles study of Pt adhesion and growth on SrO- and TiO2-terminated SrTiO3(100). Journal of Chemical Physics, 2002, 116, 9914-9925.	3.0	74
13	Molecular adsorption of small alkanes on a PdO(101) thin film: Evidence of Ïƒ-complex formation. Journal of Chemical Physics, 2010, 132, 024709.	3.0	71
14	A First-Principles Study of the Role of Quaternary-N Doping on the Oxygen Reduction Reaction Activity and Selectivity of Graphene Edge Sites. Topics in Catalysis, 2013, 56, 1623-1633.	2.8	67
15	Atomically Detailed Models of the Effect of Thermal Roughening on the Enantiospecificity of Naturally Chiral Platinum Surfaces. Langmuir, 2002, 18, 3737-3748.	3.5	66
16	Dispersion-corrected density functional theory calculations of the molecular binding of n-alkanes on Pd(111) and PdO(101). Journal of Chemical Physics, 2012, 136, 054702.	3.0	65
17	Density Functional Theory Study of Methanol Steam Reforming on Co(0001) and Co(111) Surfaces. Journal of Physical Chemistry C, 2014, 118, 15274-15285.	3.1	65
18	Poisoning effect of adsorbed CO during CO₂ electroreduction on late transition metals. Physical Chemistry Chemical Physics, 2014, 16, 20429-20435.	2.8	63

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19	First-principles study of cubic Bi pyrochlores. Physical Review B, 2008, 77, .	3.2	61
20	Thin Pt films on the polar SrTiO3(111) surface: an experimental and theoretical study. Surface Science, 2003, 537, 134-152.	1.9	60
21	Adsorption of Water on a PdO(101) Thin Film: Evidence of an Adsorbed HOâ¯H2O Complex. Journal of Physical Chemistry C, 2009, 113, 1495-1506.	3.1	59
22	CO Poisoning Effects on FeNC and CN_x ORR Catalysts: A Combined Experimentalâ€“Computational Study. Journal of Physical Chemistry C, 2016, 120, 15173-15184.	3.1	57
23	Theoretical insight on reactivity trends in CO₂ electroreduction across transition metals. Catalysis Science and Technology, 2016, 6, 1042-1053.	4.1	57
24	Precursor-mediated dissociation of n-butane on a PdO(101) thin film. Catalysis Today, 2011, 160, 213-227.	4.4	55
25	Facile Dehydrogenation of Ethane on the IrO₂(110) Surface. Journal of the American Chemical Society, 2018, 140, 2665-2672.	13.7	55
26	Pathways and kinetics of methane and ethane Câ€“H bond cleavage on PdO(101). Journal of Chemical Physics, 2013, 139, 104702.	3.0	49
27	Surface phases of Cu2O(111) under CO2 electrochemical reduction conditions. Catalysis Communications, 2014, 52, 88-91.	3.3	49
28	Structure and energetics of 180Â° domain walls in PbTiO₃by density functional theory. Journal of Physics Condensed Matter, 2011, 23, 175902.	1.8	48
29	Strong Kinetic Isotope Effect in the Dissociative Chemisorption of H₂ on a PdO(101) Thin Film. Journal of Physical Chemistry C, 2010, 114, 11485-11497.	3.1	47
30	Alkane Activation and Oxidation on Late-Transition-Metal Oxides: Challenges and Opportunities. ACS Catalysis, 2021, 11, 4682-4703.	11.2	47
31	Thermal Fluctuations in the Structure of Naturally Chiral Pt surfaces. Topics in Catalysis, 2002, 18, 193-200.	2.8	44
32	Atomistic Model Potential for PbTiO3and PMN by Fitting First Principles Results. Ferroelectrics, 2004, 301, 55-59.	0.6	42
33	DFT study of Pt adsorption on low index SrTiO3 surfaces: SrTiO3(100), SrTiO3(111) and SrTiO3(110). Surface Science, 2005, 581, 66-87.	1.9	41
34	CO Oxidation on PdO(101) during Temperature-Programmed Reaction Spectroscopy: Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2014, 118, 28647-28661.	3.1	40
35	Vacancy-Mediated Processes in the Oxidation of CO on PdO(101). Accounts of Chemical Research, 2015, 48, 1515-1523.	15.6	39
36	Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). ACS Catalysis, 2018, 8, 8553-8567.	11.2	38

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37	Pathways for Câ€“H bond cleavage of propane Ïƒ-complexes on PdO(101). Physical Chemistry Chemical Physics, 2012, 14, 12202.	2.8	34
38	Anab initiostudy of adsorption of alanine on the chiral calcite surface. Molecular Simulation, 2007, 33, 343-351.	2.0	33
39	Adsorption of alkanes on stoichiometric and oxygen-rich RuO₂(110). Physical Chemistry Chemical Physics, 2016, 18, 22647-22660.	2.8	33
40	The role of phase impurities and lattice defects on the electron dynamics and photochemistry of CuFeO2 solar photocathodes. Nano Research, 2019, 12, 2390-2399.	10.4	31
41	Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. Annual Review of Materials Research, 2007, 37, 239-270.	9.3	29
42	CO oxidation on single and multilayer Pd oxides on Pd(111): mechanistic insights from RAIRS. Catalysis Science and Technology, 2014, 4, 3826-3834.	4.1	29
43	Kinetics of low-temperature methane activation on IrO2(1Â1Â0): Role of local surface hydroxide species. Journal of Catalysis, 2020, 383, 181-192.	6.2	29
44	High Selectivity for Primary Câ€“H Bond Cleavage of Propane Ïƒ-Complexes on the PdO(101) Surface. Journal of the American Chemical Society, 2011, 133, 16196-16200.	13.7	28
45	Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. Surface Science, 2012, 606, 1280-1288.	1.9	27
46	Growth and Structure of Cu and Au on the Nonpolar ZnO(101Ì…0) Surface: STM, XPS, and DFT Studies. Journal of Physical Chemistry C, 2013, 117, 18386-18397.	3.1	27
47	An ab initio thermodynamics study of cobalt surface phases under ethanol steam reforming conditions. Catalysis Science and Technology, 2014, 4, 3379-3389.	4.1	27
48	Dissociative Chemisorption and Oxidation of H2 on the Stoichiometric IrO2(110) Surface. Topics in Catalysis, 2018, 61, 397-411.	2.8	27
49	Adsorption and Oxidation of CH₄ on Oxygen-Rich IrO₂(110). Journal of Physical Chemistry C, 2019, 123, 27603-27614.	3.1	27
50	Dissociative Adsorption of Hydrogen on PdO(101) Studied by HRCLS and DFT. Journal of Physical Chemistry C, 2013, 117, 13510-13519.	3.1	25
51	Hole Thermalization Dynamics Facilitate Ultrafast Spatial Charge Separation in CuFeO₂ Solar Photocathodes. Journal of Physical Chemistry C, 2018, 122, 11300-11304.	3.1	25
52	Brillouin scattering and molecular dynamics study of the elastic properties ofPb(Mg1â^•3Nb2â^•3)O3. Physical Review B, 2007, 75, .	3.2	24
53	Molecular dynamics simulations of CO2 reduction on Cu(111) and Cu/ZnO(10 <mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	3.3	24
54	Adsorption and oxidation of propane and cyclopropane on IrO₂(110). Physical Chemistry Chemical Physics, 2018, 20, 29264-29273.	2.8	24

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55	Experimental and DFT Investigation into Chloride Poisoning Effects on Nitrogen-Coordinated Ironâ€“Carbon (FeNC) Catalysts for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2020, 124, 10324-10335.	3.1	23
56	Advances in First-Principles Studies of Transducer Materials. Ferroelectrics, 2006, 333, 69-78.	0.6	22
57	Pt thin films on the polarLaAlO3(100)surface: A first-principles study. Physical Review B, 2006, 73, .	3.2	22
58	A first-principles study of H2O adsorption and dissociation on the SrTiO3(100) surface. Molecular Simulation, 2010, 36, 604-617.	2.0	21
59	Propane Ïƒâ€Complexes on PdO(101): Spectroscopic Evidence of the Selective Coordination and Activation of Primary Cï£¿H Bonds. Angewandte Chemie - International Edition, 2015, 54, 13907-13911.	13.8	21
60	Adsorption and Oxidation of n-Butane on the Stoichiometric RuO₂(110) Surface. Journal of Physical Chemistry C, 2016, 120, 9863-9873.	3.1	21
61	Growth and termination of a rutile IrO2(100) layer on Ir(111). Surface Science, 2016, 652, 213-221.	1.9	21
62	Adsorption of CO₂ on a PdO(101) Thin Film. Journal of Physical Chemistry C, 2012, 116, 3007-3016.	3.1	20
63	Adsorption and Oxidation of Ethylene on the Stoichiometric and O-Rich RuO₂(110) Surfaces. Journal of Physical Chemistry C, 2017, 121, 20375-20386.	3.1	18
64	Cu cluster deposition on ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si10.gif" overflow="scroll"><mml:mfenced open="(") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 392 Td (close=")"><mml:mrow><mml:mn accent="true"><mml:mn>1</mml:mn><mml:mo stretchy="true">Â¯</mml:mo></mml:mover><mml:mn>0</mml:mn></mml:mrow></mml:mfenced></mml:math>: Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014,	1.9	16
65	Hydrogen oxidation on oxygen-rich IrO₂(110). Journal of Lithic Studies, 2018, 4, 1-13.	0.5	16
66	STM and DFT studies of CO2 adsorption on O-Cu(100) surface. Surface Science, 2019, 679, 50-55.	1.9	15
67	Molecular chemisorption of N2 on IrO2(110). Journal of Chemical Physics, 2020, 152, 074712.	3.0	15
68	Selectivity in the initial Câ€“H bond cleavage of n-butane on PdO(101). Physical Chemistry Chemical Physics, 2013, 15, 12075.	2.8	14
69	High-Resolution X-ray Photoelectron Spectroscopy of an IrO₂(110) Film on Ir(100). Journal of Physical Chemistry Letters, 2020, 11, 7184-7189.	4.6	14
70	Catalytic Oxidation of Methane on IrO₂(110) Films Investigated Using Ambient-Pressure X-ray Photoelectron Spectroscopy. ACS Catalysis, 2022, 12, 2840-2853.	11.2	14
71	A first-principles study of Pt thin films on SrTiO3(100): Support effects on CO adsorption. Journal of Chemical Physics, 2015, 142, 124704.	3.0	13
72	Initial Reduction of the PdO(101) Surface: Role of Oxygen Vacancy Formation Kinetics. Journal of Physical Chemistry C, 2018, 122, 26007-26017.	3.1	13

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73	Single-domain electromechanical constants for Pb(Zn1â^•3Nb2â^•3)O3â€“4.5%PbTiO3 from micro-Brillouin scattering. Applied Physics Letters, 2006, 88, 042908.	3.3	12
74	Coupling of surface relaxation and polarization in PbTiO₃from atomistic simulation. Journal of Physics Condensed Matter, 2008, 20, 395004.	1.8	12
75	Changes in Active Sites on Nitrogenâ€Doped Carbon Catalysts Under Oxygen Reduction Reaction: A Combined Postâ€Reaction Characterization and DFT Study. ChemCatChem, 2019, 11, 5945-5950.	3.7	12
76	Isothermal Reduction of IrO₂(110) Films by Methane Investigated Using In Situ X-ray Photoelectron Spectroscopy. ACS Catalysis, 2021, 11, 5004-5016.	11.2	12
77	Pt thin films on stepped SrTiO3 surfaces: SrTiO3(620) and SrTiO3(622). Journal of Molecular Catalysis A, 2004, 216, 233-245.	4.8	11
78	Capturing dynamic cation hopping in cubic pyrochlores. Applied Physics Letters, 2011, 99, .	3.3	10
79	First Principles Study of Molecular O2 Adsorption on the PdO(101) Surface. Topics in Catalysis, 2017, 60, 401-412.	2.8	9
80	Ensemble effects in Cu/Au ultrasmall nanoparticles control the branching point for C1 selectivity during CO₂ electroreduction. Chemical Science, 2021, 12, 9146-9152.	7.4	9
81	Energy landscape in frustrated systems: Cation hopping in pyrochlores. Applied Physics Letters, 2013, 103, 022901.	3.3	6
82	Molecular adsorption of NO on PdO(101). Surface Science, 2015, 640, 150-158.	1.9	6
83	Promotion of CO oxidation on PdO(101) by adsorbed H2O. Surface Science, 2016, 650, 203-209.	1.9	6
84	A first-principles study of methyl lactate adsorption on the chiral Cu (643) surface. Surface Science, 2014, 629, 28-34.	1.9	4
85	Water adsorption on olivine(010) surfaces: Effect of alkali and transition metal cation doping. Journal of Chemical Physics, 2019, 150, 044703.	3.0	4
86	The influence of sulfur substitution on the atomic displacement in Bi2Ti2O7. Journal of Solid State Chemistry, 2010, 183, 262-269.	2.9	3
87	Publisher's Note: Second-generation charge-optimized many-body potential for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext> amorphous silica [Phys. Rev. B82, 235302 (2010)]. Physical Review B, 2010, 82, .	3.2	3
88	Brillouin spectroscopy of relaxor ferroelectrics and metal hydrides. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 442, 519-522.	5.6	1
89	Tunable tunnel barriers in a semiconductor via ionization of individual atoms. Journal of Physics Condensed Matter, 2021, 33, 275002.	1.8	1
90	Catalytic Chemistry on Oxide Nanostructures. Springer Series in Materials Science, 2016, , 251-280.	0.6	0