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	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
2	Alkane Activation and Oxidation on Late-Transition-Metal Oxides: Challenges and Opportunities. ACS Catalysis, 2021, 11, 4682-4703.	11.2	47
3	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
4	Tunable tunnel barriers in a semiconductor via ionization of individual atoms. Journal of Physics Condensed Matter, 2021, 33, 275002.	1.8	1
5	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
6	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
7	Molecular chemisorption of N2 on IrO2(110). Journal of Chemical Physics, 2020, 152, 074712.	3.0	15
8	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
9	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
10	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
11	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
12	Adsorption and Oxidation of CH₄ on Oxygen-Rich IrO₂(110). Journal of Physical Chemistry C, 2019, 123, 27603-27614.	3.1	27
13	Water adsorption on olivine(010) surfaces: Effect of alkali and transition metal cation doping. Journal of Chemical Physics, 2019, 150, 044703.	3.0	4
14	STM and DFT studies of CO2 adsorption on O-Cu(100) surface. Surface Science, 2019, 679, 50-55.	1.9	15
15	Solvation effects on DFT predictions of ORR activity on metal surfaces. Catalysis Today, 2019, 323, 35-43.	4.4	109
16	Facile Dehydrogenation of Ethane on the IrO₂(110) Surface. Journal of the American Chemical Society, 2018, 140, 2665-2672.	13.7	55
17	Dissociative Chemisorption and Oxidation of H2 on the Stoichiometric IrO2(110) Surface. Topics in Catalysis, 2018, 61, 397-411.	2.8	27
18	Hydrogen oxidation on oxygen-rich IrO₂(110). Journal of Lithic Studies, 2018, 4, 1-13.	0.5	16

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19	Adsorption and oxidation of propane and cyclopropane on IrO₂(110). Physical Chemistry Chemical Physics, 2018, 20, 29264-29273.	2.8	24
20	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
21	Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). ACS Catalysis, 2018, 8, 8553-8567.	11.2	38
22	Hole Thermalization Dynamics Facilitate Ultrafast Spatial Charge Separation in CuFeO₂ Solar Photocathodes. Journal of Physical Chemistry C, 2018, 122, 11300-11304.	3.1	25
23	Low-temperature activation of methane on the IrO ₂ (110) surface. Science, 2017, 356, 299-303.	12.6	244
24	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
25	First Principles Study of Molecular O2 Adsorption on the PdO(101) Surface. Topics in Catalysis, 2017, 60, 401-412.	2.8	9
26	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
27	Adsorption and Oxidation of n-Butane on the Stoichiometric RuO₂(110) Surface. Journal of Physical Chemistry C, 2016, 120, 9863-9873.	3.1	21
28	Catalytic Chemistry on Oxide Nanostructures. Springer Series in Materials Science, 2016, , 251-280.	0.6	0
29	Adsorption of alkanes on stoichiometric and oxygen-rich RuO₂(110). Physical Chemistry Chemical Physics, 2016, 18, 22647-22660.	2.8	33
30	Growth and termination of a rutile IrO2(100) layer on Ir(111). Surface Science, 2016, 652, 213-221.	1.9	21
31	Facet Dependence of CO₂ Reduction Paths on Cu Electrodes. ACS Catalysis, 2016, 6, 219-229.	11.2	420
32	Promotion of CO oxidation on PdO(101) by adsorbed H2O. Surface Science, 2016, 650, 203-209.	1.9	6
33	Theoretical insight on reactivity trends in CO₂ electroreduction across transition metals. Catalysis Science and Technology, 2016, 6, 1042-1053.	4.1	57
34	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
35	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
36	Molecular adsorption of NO on PdO(101). Surface Science, 2015, 640, 150-158.	1.9	6

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37	Vacancy-Mediated Processes in the Oxidation of CO on PdO(101). Accounts of Chemical Research, 2015, 48, 1515-1523.	15.6	39
38	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
39	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
40	Alkane activation on crystalline metal oxide surfaces. Chemical Society Reviews, 2014, 43, 7536-7547.	38.1	133
41	A first-principles study of methyl lactate adsorption on the chiral Cu (643) surface. Surface Science, 2014, 629, 28-34.	1.9	4
42	Molecular dynamics simulations of CO2 reduction on Cu(111) and Cu/ZnO(10 <mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 552 Td (altimg="si10.gif" overflow="scroll"><mml:mfenced open="(") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 512 Td (close=")"><mml:mover 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>: Cu cluster deposition on ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014,	3.3	24
43		1.9	16
44	Poisoning effect of adsorbed CO during CO₂ electroreduction on late transition metals. Physical Chemistry Chemical Physics, 2014, 16, 20429-20435.	2.8	63
45	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
46	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
47	Reaction mechanisms of CO2 electrochemical reduction on Cu(111) determined with density functional theory. Journal of Catalysis, 2014, 312, 108-122.	6.2	382
48	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
49	Surface phases of Cu2O(111) under CO2 electrochemical reduction conditions. Catalysis Communications, 2014, 52, 88-91.	3.3	49
50	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
51	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
52	Selectivity in the initial Câ€“H bond cleavage of n-butane on PdO(101). Physical Chemistry Chemical Physics, 2013, 15, 12075.	2.8	14
53	Dissociative Adsorption of Hydrogen on PdO(101) Studied by HRCLS and DFT. Journal of Physical Chemistry C, 2013, 117, 13510-13519.	3.1	25
54	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

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55	Pathways and kinetics of methane and ethane Câ€“H bond cleavage on PdO(101). Journal of Chemical Physics, 2013, 139, 104702.	3.0	49
56	Energy landscape in frustrated systems: Cation hopping in pyrochlores. Applied Physics Letters, 2013, 103, 022901.	3.3	6
57	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
58	Pathways for Câ€“H bond cleavage of propane Ïƒ-complexes on PdO(101). Physical Chemistry Chemical Physics, 2012, 14, 12202.	2.8	34
59	Adsorption of CO₂ on a PdO(101) Thin Film. Journal of Physical Chemistry C, 2012, 116, 3007-3016.	3.1	20
60	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
61	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
62	Precursor-mediated dissociation of n-butane on a PdO(101) thin film. Catalysis Today, 2011, 160, 213-227.	4.4	55
63	Structure and energetics of 180Â° domain walls in PbTiO₃by density functional theory. Journal of Physics Condensed Matter, 2011, 23, 175902.	1.8	48
64	Capturing dynamic cation hopping in cubic pyrochlores. Applied Physics Letters, 2011, 99, .	3.3	10
65	The influence of sulfur substitution on the atomic displacement in Bi2Ti2O7. Journal of Solid State Chemistry, 2010, 183, 262-269.	2.9	3
66	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
67	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></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> amorphous silica [Phys. Rev. B82, 235302 (2010)]. Physical Review B, 2010, 82, .	3.2	3
68	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
69	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></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> amorphous silica. Physical Review B, 2010, 82, .	3.2	90
70	A first-principles study of H2O adsorption and dissociation on the SrTiO3(100) surface. Molecular Simulation, 2010, 36, 604-617.	2.0	21
71	Density functional theory study of the initial oxidation of the Pt(111) surface. Physical Review B, 2009, 79, .	3.2	96
72	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

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73	First-principles study of cubic Bi pyrochlores. Physical Review B, 2008, 77, .	3.2	61
74	Coupling of surface relaxation and polarization in PbTiO₃from atomistic simulation. Journal of Physics Condensed Matter, 2008, 20, 395004.	1.8	12
75	Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. Annual Review of Materials Research, 2007, 37, 239-270.	9.3	29
76	Brillouin scattering and molecular dynamics study of the elastic properties ofPb(Mg1âˆ•3Nb2âˆ•3)O3. Physical Review B, 2007, 75, .	3.2	24
77	Anab initiostudy of adsorption of alanine on the chiral calcite surface. Molecular Simulation, 2007, 33, 343-351.	2.0	33
78	Advances in First-Principles Studies of Transducer Materials. Ferroelectrics, 2006, 333, 69-78.	0.6	22
79	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
80	Single-domain electromechanical constants for Pb(Zn1âˆ•3Nb2âˆ•3)O3â€“4.5%PbTiO3 from micro-Brillouin scattering. Applied Physics Letters, 2006, 88, 042908.	3.3	12
81	Pt thin films on the polarLaAlO3(100)surface: A first-principles study. Physical Review B, 2006, 73, .	3.2	22
82	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
83	Atomic-level simulation of ferroelectricity in oxide materials. Current Opinion in Solid State and Materials Science, 2005, 9, 107-113.	11.5	109
84	Pt thin films on stepped SrTiO3 surfaces: SrTiO3(620) and SrTiO3(622). Journal of Molecular Catalysis A, 2004, 216, 233-245.	4.8	11
85	Atomistic Model Potential for PbTiO3and PMN by Fitting First Principles Results. Ferroelectrics, 2004, 301, 55-59.	0.6	42
86	Thin Pt films on the polar SrTiO3(111) surface: an experimental and theoretical study. Surface Science, 2003, 537, 134-152.	1.9	60
87	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
88	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
89	Thermal Fluctuations in the Structure of Naturally Chiral Pt surfaces. Topics in Catalysis, 2002, 18, 193-200.	2.8	44
90	Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents. Journal of Physical Chemistry B, 2001, 105, 4771-4782.	2.6	203