Horia Metiu

List of Publications by Year
in descending order

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336 papers	17,526 citations	11608 70 h-index	22102 113 g-index

343 all docs	343 docs citations	343 times ranked	11575 citing authors

#	Article	IF	Citations
1	Influence of hydrocarbon feed additives on the high-temperature pyrolysis of methane in molten salt bubble column reactors. Reaction Chemistry and Engineering, 2022, 7, 1199-1209.	1.9	7
2	Properties of Methane and Carbon Adsorbed at the Interface between Molten NaBr and Ni(111). Journal of Physical Chemistry C, 2021, 125, 3980-3987.	1.5	3
3	Initial Steps in CH₄ Pyrolysis on Cu and Ni. Journal of Physical Chemistry C, 2021, 125, 18665-18672.	1.5	4
4	Methane pyrolysis in low-cost, alkali-halide molten salts at high temperatures. Sustainable Energy and Fuels, 2021, 5, 6107-6123.	2.5	31
5	Molecular Oxygen Activation on Suspended Doped Cerium(IV) Oxide Particles in Molten Chloride Salts. Catalysis Letters, 2020, 150, 273-280.	1.4	1
6	Catalytic Methane Pyrolysis with Liquid and Vapor Phase Tellurium. ACS Catalysis, 2020, 10, 8223-8230.	5.5	42
7	CO₂-Free Hydrogen Production by Catalytic Pyrolysis of Hydrocarbon Feedstocks in Molten Niâ€“Bi. Energy & Fuels, 2020, 34, 16073-16080.	2.5	40
8	Catalytic Methane Pyrolysis in Molten Alkali Chloride Salts Containing Iron. ACS Catalysis, 2020, 10, 7032-7042.	5.5	59
9	High-temperature heterogeneous catalysis in platinum nanoparticle â€“ molten salt suspensions. Catalysis Science and Technology, 2020, 10, 625-629.	2.1	5
10	Dry reforming of methane catalysed by molten metal alloys. Nature Catalysis, 2020, 3, 83-89.	16.1	153
11	Oxide Catalysts. , 2020, , 1343-1354.		1
12	Rates of adsorption and desorption: Entropic contributions and errors due to mean-field approximations. Journal of Chemical Physics, 2019, 150, 184702.	1.2	5
13	Methane Pyrolysis with a Molten Cuâ€“Bi Alloy Catalyst. ACS Catalysis, 2019, 9, 8337-8345.	5.5	112
14	Properties of Negatively Charged Ruthenium Clusters in Molten Sodium Chloride. Journal of Physical Chemistry C, 2019, 123, 16179-16185.	1.5	5
15	Catalytic methane pyrolysis in molten MnCl2-KCl. Applied Catalysis B: Environmental, 2019, 254, 659-666.	10.8	104
16	Solid carbon production and recovery from high temperature methane pyrolysis in bubble columns containing molten metals and molten salts. Carbon, 2019, 151, 181-191.	5.4	95
17	Bromine and iodine for selective partial oxidation of propane and methane. Applied Catalysis A: General, 2019, 580, 102-110.	2.2	8
18	Halogen-Mediated Partial Combustion of Methane in Molten Salts To Produce CO₂-Free Power and Solid Carbon. ACS Sustainable Chemistry and Engineering, 2018, 6, 15673-15681.	3.2	9

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19	Chlorine Production by HCl Oxidation in a Molten Chloride Salt Catalyst. Industrial & Engineering Chemistry Research, 2018, 57, 7795-7801.	1.8	4
20	Oxide Catalysts. , 2018, , 1-12.		0
21	Chemistry of Solvated Electrons in Molten Alkali Chloride Salts. Journal of Physical Chemistry C, 2018, 122, 19603-19612.	1.5	11
22	Molten salt chemical looping for reactive separation of HBr in a halogen-based natural gas conversion process. Chemical Engineering Science, 2017, 160, 245-253.	1.9	11
23	Stability of V₂O₅ Supported on Titania in the Presence of Water, Bulk Oxygen Vacancies, and Adsorbed Oxygen Atoms. Journal of Physical Chemistry C, 2017, 121, 8444-8451.	1.5	13
24	Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon. Science, 2017, 358, 917-921.	6.0	306
25	Reactions of Molten LiI with I₂, H₂O, and O₂ Relevant to Halogen-Mediated Oxidative Dehydrogenation of Alkanes. Journal of Physical Chemistry C, 2016, 120, 4931-4936.	1.5	6
26	Structure and Oxidizing Power of Single Layer Î±-V2O5. Topics in Catalysis, 2016, 59, 809-816.	1.3	6
27	Partial oxidation of propane with CO₂ on Ru doped catalysts. Catalysis Science and Technology, 2016, 6, 5483-5493.	2.1	17
28	Oxygen Vacancy Formation on Î±-MoO₃ Slabs and Ribbons. Journal of Physical Chemistry C, 2016, 120, 19252-19264.	1.5	44
29	Doped rhodium sulfide and thiospinels hydrogen evolution and oxidation electrocatalysts in strong acid electrolytes. Journal of Applied Electrochemistry, 2016, 46, 497-503.	1.5	12
30	Interaction between Monomeric Vanadium Oxide Clusters Supported on Titania and Its Influence on Their Reactivity. Journal of Physical Chemistry C, 2016, 120, 13610-13621.	1.5	10
31	Energy of Oxygen-Vacancy Formation on Oxide Surfaces: Role of the Spatial Distribution. Journal of Physical Chemistry C, 2016, 120, 2320-2323.	1.5	21
32	Structure of V₂O₅Â·nH₂O Xerogels. Journal of Physical Chemistry C, 2016, 120, 3986-3992.	1.5	68
33	Halogen-Mediated Oxidative Dehydrogenation of Propane Using Iodine or Molten Lithium Iodide. Catalysis Letters, 2016, 146, 744-754.	1.4	8
34	Catechol and HCl Adsorption on TiO₂(110) in Vacuum and at the Waterâ€“TiO₂ Interface. Journal of Physical Chemistry Letters, 2015, 6, 2277-2281.	2.1	32
35	Reconstruction of Low-Index Î±-V₂O₅ Surfaces. Journal of Physical Chemistry C, 2015, 119, 10500-10506.	1.5	12
36	Hydrogen Abstraction Energies and Ammonia Binding to BEA, ZSM-5, and Î±-Quartz Doped with Al, Sc, B, or Ga. Journal of Physical Chemistry C, 2015, 119, 16106-16114.	1.5	11

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37	Molten LiCl Layer Supported on MgO: Its Possible Role in Enhancing the Oxidative Dehydrogenation of Ethane. Journal of Physical Chemistry C, 2015, 119, 8681-8691.	1.5	18
38	CO₂methanation by Ru-doped ceria: the role of the oxidation state of the surface. Catalysis Science and Technology, 2015, 5, 1783-1791.	2.1	96
39	Hydrogen Dissociative Adsorption on Lanthana: Polaron Formation and the Role of Acidâ€“Base Interactions. Journal of Physical Chemistry C, 2015, 119, 19876-19882.	1.5	22
40	Acidâ€“Base Interaction and Its Role in Alkane Dissociative Chemisorption on Oxide Surfaces. Journal of Physical Chemistry C, 2014, 118, 27336-27342.	1.5	54
41	Stable electrocatalysts for autonomous photoelectrolysis of hydrobromic acid using single-junction solar cells. Energy and Environmental Science, 2014, 7, 978-981.	15.6	17
42	Catalytic Oxidation of Methanol to Formaldehyde by Mass-Selected Vanadium Oxide Clusters Supported on a TiO₂(110) Surface. Journal of Physical Chemistry A, 2014, 118, 8309-8313.	1.1	19
43	Investigation of the Electrocatalytic Activity of Rhodium Sulfide for Hydrogen Evolution and Hydrogen Oxidation. Electrochimica Acta, 2014, 145, 224-230.	2.6	25
44	Investigation of the Active Sites of Rhodium Sulfide for Hydrogen Evolution/Oxidation Using Carbon Monoxide as a Probe. Langmuir, 2014, 30, 5662-5668.	1.6	7
45	Oxygen Adsorption on Irreducible Oxides Doped with Higher Valence Ions: O₂ Binding to the Dopant. Journal of Physical Chemistry C, 2014, 118, 23070-23082.	1.5	5
46	Catalytic Dry Reforming of Methane on Ruthenium-Doped Ceria and Ruthenium Supported on Ceria. Topics in Catalysis, 2014, 57, 118-124.	1.3	38
47	Ethane Activation by Nb-Doped NiO. Journal of Physical Chemistry C, 2013, 117, 23597-23608.	1.5	26
48	Methane Oxidation by Lanthanum Oxide Doped with Cu, Zn, Mg, Fe, Nb, Ti, Zr, or Ta: The Connection Between the Activation Energy and the Energy of Oxygen-Vacancy Formation. Catalysis Letters, 2013, 143, 406-410.	1.4	37
49	The Selective High-Yield Conversion of Methane Using Iodine-Catalyzed Methane Bromination. ACS Catalysis, 2013, 3, 474-477.	5.5	26
50	Catalysis by Doped Oxides. Chemical Reviews, 2013, 113, 4391-4427.	23.0	687
51	Transition Metal Sulfide Hydrogen Evolution Catalysts for Hydrobromic Acid Electrolysis. Langmuir, 2013, 29, 480-492.	1.6	81
52	Interplay Between Bromine and Iodine in Oxidative Dehydrogenation. ChemCatChem, 2013, 5, 1906-1910.	1.8	22
53	Methane Dissociation on Li-, Na-, K-, and Cu-Doped Flat and Stepped CaO(001). Journal of Physical Chemistry C, 2013, 117, 7114-7122.	1.5	24
54	Oxidative Dehydrogenation of Methane by Isolated Vanadium Oxide Clusters Supported on Au (111) and Ag (111) Surfaces. Journal of Physical Chemistry C, 2013, 117, 18475-18483.	1.5	8

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55	Gas-Phase Chemistry to Understand Electrochemical Hydrogen Evolution and Oxidation on Doped Transition Metal Sulfides. Journal of the Electrochemical Society, 2013, 160, A1902-A1906.	1.3	5
56	Preface: Special Topic Section on Photochemistry at Surfaces. Journal of Chemical Physics, 2012, 137, 091501.	1.2	1
57	Hydrodebromination and Oligomerization of Dibromomethane. ACS Catalysis, 2012, 2, 479-486.	5.5	28
58	Does Halogen Adsorption Activate the Oxygen Atom on an Oxide Surface? I. A Study of Br₂ and HBr Adsorption on La₂O₃ and La₂O₃ Doped with Mg or Zr. Journal of Physical Chemistry C, 2012, 116, 4137-4148.	1.5	20
59	Halogen Adsorption on CeO₂: The Role of Lewis Acidâ€“Base Pairing. Journal of Physical Chemistry C, 2012, 116, 6664-6671.	1.5	48
60	DFT Study of the Electronic Properties of LaOCl Surfaces. Journal of Physical Chemistry C, 2012, 116, 681-691.	1.5	13
61	Chemistry of Lewis Acidâ€“Base Pairs on Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 10439-10450.	1.5	293
62	Dissociation of Methane on La₂O₃ Surfaces Doped with Cu, Mg, or Zn. Journal of Physical Chemistry C, 2011, 115, 18239-18246.	1.5	31
63	Effect of Dopants on the Energy of Oxygen-Vacancy Formation at the Surface of Ceria: Local or Global?. Journal of Physical Chemistry C, 2011, 115, 17898-17909.	1.5	118
64	Câ€“H Bond Activation by Pd-substituted CeO₂: Substituted Ions versus Reduced Species. Chemistry of Materials, 2011, 23, 5432-5439.	3.2	35
65	Choice of U for DFT+U Calculations for Titanium Oxides. Journal of Physical Chemistry C, 2011, 115, 5841-5845.	1.5	264
66	Chemistry of Doped Oxides: The Activation of Surface Oxygen and the Chemical Compensation Effect. Journal of Physical Chemistry C, 2011, 115, 3065-3074.	1.5	102
67	CO2 methanation on Ru-doped ceria. Journal of Catalysis, 2011, 278, 297-309.	3.1	328
68	Electronic Structure of Partially Reduced Rutile TiO₂(110) Surface: Where Are the Unpaired Electrons Located?. Journal of Physical Chemistry C, 2011, 115, 4696-4705.	1.5	153
69	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO₂(110) by Transitionâ€Metal Substitution. ChemCatChem, 2011, 3, 1607-1611.	1.8	169
70	STM characterization of size-selected V1, V2, VO, and VO2 clusters on a TiO2(110)-(1Ã—1) surface at room temperature. Surface Science, 2011, 605, 972-976.	0.8	27
71	Methane complete and partial oxidation catalyzed by Pt-doped CeO2. Journal of Catalysis, 2010, 273, 125-137.	3.1	186
72	Oxidative Dehydrogenation of Methanol to Formaldehyde by a Vanadium Oxide Cluster Supported on Rutile TiO₂(110): Which Oxygen is Involved?. Journal of Physical Chemistry C, 2010, 114, 13736-13738.	1.5	30

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73	DFT Studies of Oxygen Vacancies on Undoped and Doped La₂O₃ Surfaces. Journal of Physical Chemistry C, 2010, 114, 12234-12244.	1.5	101
74	Direct Visualization of Water-Induced Relocation of Au Atoms from Oxygen Vacancies on a TiO₂(110) Surface. Journal of Physical Chemistry C, 2010, 114, 3987-3990.	1.5	40
75	CO oxidation by Ti- and Al-doped ZnO: Oxygen activation by adsorption on the dopant. Journal of Catalysis, 2009, 266, 50-58.	3.1	58
76	Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. Surface Science, 2009, 603, 1724-1730.	0.8	99
77	Oxidative Dehydrogenation of Methanol to Formaldehyde by Isolated Vanadium, Molybdenum, and Chromium Oxide Clusters Supported on Rutile TiO2(110). Journal of Physical Chemistry C, 2009, 113, 16083-16093.	1.5	38
78	Size and pressure independent kinetics of CO oxidation on aluminaâ€supported iridium nanoparticles. International Journal of Chemical Kinetics, 2008, 40, 826-830.	1.0	5
79	Vacancy formation and CO adsorption on gold-doped ceria surfaces. Surface Science, 2008, 602, 2734-2742.	0.8	125
80	Selective promotion of different modes of methanol adsorption via the cation substitutional doping of a ZnO(101Â¯0) surface. Journal of Catalysis, 2008, 254, 325-331.	3.1	38
81	O 2 evolution on a clean partially reduced rutile TiO2(110) surface and on the same surface precovered with Au1 and Au2: The importance of spin conservation. Journal of Chemical Physics, 2008, 129, 074705.	1.2	113
82	Enhanced adsorption energy of Au1 and O2 on the stoichiometric TiO2(110) surface by coadsorption with other molecules. Journal of Chemical Physics, 2008, 128, 044714.	1.2	54
83	CO Oxidation by Rutile TiO₂(110) Doped with V, W, Cr, Mo, and Mn. Journal of Physical Chemistry C, 2008, 112, 12398-12408.	1.5	115
84	Inelastic Scattering with Chebyshev Polynomials and Preconditioned Conjugate Gradient Minimization. Journal of Physical Chemistry A, 2008, 112, 2728-2737.	1.1	0
85	Preface to Special Topic: A Survey of Some New Developments in Heterogeneous Catalysis. Journal of Chemical Physics, 2008, 128, 182501.	1.2	20
86	Density functional study of the interaction between small Au clusters, Aunâ€ˆ(n=1â€“7) and the rutile TiO2 surface. II. Adsorption on a partially reduced surface. Journal of Chemical Physics, 2007, 127, 244708.	1.2	52
87	Density functional study of the charge on Aun clusters (n=1â€“7) supported on a partially reduced rutile TiO2(110): Are all clusters negatively charged?. Journal of Chemical Physics, 2007, 126, 104701.	1.2	72
88	Catalysis by very small Au clusters. Current Opinion in Solid State and Materials Science, 2007, 11, 62-75.	5.6	113
89	VO_x (x = 1â^'4) Submonolayers Supported on Rutile TiO₂(110) and CeO₂(111) Surfaces:â€‰ The Structure, the Charge of the Atoms, the XPS Spectrum, and the Equilibrium Composition in the Presence of Oxygen. Journal of Physical Chemistry C, 2007, 111, 14179-14188.	1.5	47
90	Dynamics of H2O and Na+in Nafion Membranes. Journal of Physical Chemistry B, 2007, 111, 2490-2494.	1.2	53

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91	Nanoscale Current Imaging of the Conducting Channels in Proton Exchange Membrane Fuel Cells. Nano Letters, 2007, 7, 227-232.	4.5	84
92	Modification of the Oxidative Power of ZnO(101Ì„0) Surface by Substituting Some Surface Zn Atoms with Other Metals. Journal of Physical Chemistry C, 2007, 111, 8617-8622.	1.5	61
93	The Structure and Energy of Oxygen Vacancy Formation in Clean and Doped, Very Thin Films of ZnO. Journal of Physical Chemistry C, 2007, 111, 12715-12722.	1.5	30
94	Segregation at the surface of an Au/Pd alloy exposed to CO. Surface Science, 2007, 601, 5332-5339.	0.8	84
95	Catalysis by doped oxides: CO oxidation by AuxCe1âˆ’xO2. Journal of Catalysis, 2007, 245, 205-214.	3.1	325
96	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. Journal of Chemical Physics, 2007, 126, 204711.	1.2	120
97	Efficient Electrocatalyst Utilization:Â Electrochemical Deposition of Pt Nanoparticles Using Nafion Membrane as a Template. Journal of Physical Chemistry B, 2006, 110, 7119-7121.	1.2	20
98	Minimum-Error Method for Scattering Problems in Quantum Mechanics:Â Two Stable and Efficient Implementations. Journal of Physical Chemistry A, 2006, 110, 10513-10520.	1.1	3
99	Pinning Mononuclear Au on the Surface of Titania. Journal of Physical Chemistry B, 2006, 110, 663-666.	1.2	23
100	Formation, deposition and examination of size selected metal clusters on semiconductor surfaces: An experimental setup. International Journal of Mass Spectrometry, 2006, 254, 202-209.	0.7	30
101	Density Functional Study of the CO Oxidation on a Doped Rutile TiO2(110): Effect of Ionic Au in Catalysis. Catalysis Letters, 2006, 107, 143-147.	1.4	107
102	The nucleation sites of Ag clusters grown by vapor deposition on a TiO2(110)-1Ã—1 surface. Surface Science, 2005, 575, 60-68.	0.8	32
103	The binding of the noble metal cations Au+ and Ag+ to propene. Chemical Physics Letters, 2005, 412, 416-419.	1.2	8
104	Preface: Recent developments in density functional theory: Orbital dependent functionals. Journal of Chemical Physics, 2005, 123, 062101.	1.2	1
105	Pinning mass-selected Agn clusters on the TiO2(110)â˜†1Ã—1 surface via deposition at high kinetic energy. Journal of Chemical Physics, 2005, 123, 204701.	1.2	28
106	Landing of size-selected Agn+ clusters on single crystal TiO2 (110)-(1Ã—1) surfaces at room temperature. Journal of Chemical Physics, 2005, 122, 081102.	1.2	59
107	Structure of Hydrated Naâ˜†Nafion Polymer Membranes. Journal of Physical Chemistry B, 2005, 109, 24244-24253.	1.2	65
108	Electrolithographic Investigations of the Hydrophilic Channels in Nafion Membranes. Journal of Physical Chemistry B, 2005, 109, 3252-3256.	1.2	33

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109	Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?. Journal of the American Chemical Society, 2005, 127, 1049-1052.	6.6	207
110	Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion. Journal of Physical Chemistry B, 2005, 109, 3727-3730.	1.2	122
111	Intact Size-Selected AunClusters on a TiO2(110)-(1 Ã— 1) Surface at Room Temperature. Journal of the American Chemical Society, 2005, 127, 13516-13518.	6.6	136
112	Electronic states of linear Au clusters supported on metal surfaces: Why are they like those of a particle in a box?. Journal of Chemical Physics, 2004, 120, 7738-7740.	1.2	9
113	Binding of propene on small gold clusters and on Au(111): Simple rules for binding sites and relative binding energies. Journal of Chemical Physics, 2004, 121, 3756-3766.	1.2	94
114	Density functional study of the adsorption of propene on silver clusters, Agmq (m=1â€“5; q=0, +1). Journal of Chemical Physics, 2004, 121, 9925-9930.	1.2	41
115	A study of the reactions of molecular hydrogen with small gold clusters. Journal of Chemical Physics, 2004, 120, 5169-5175.	1.2	95
116	Density functional study of the adsorption of propene on mixed gold-silver clusters, AunAgm: Propensity rules for binding. Journal of Chemical Physics, 2004, 121, 9931-9937.	1.2	58
117	Reply to a comment: oxygen adsorption on Au clusters by W.T. Wallace, A.J. Leavitt, and R.J. Whetten. Chemical Physics Letters, 2003, 368, 778-779.	1.2	14
118	Adsorption of gold on stoichiometric and reduced rutile TiO2â€,(110) surfaces. Journal of Chemical Physics, 2003, 118, 6536-6551.	1.2	202
119	Oxygen adsorption on Au clusters and a rough Au(111) surface: The role of surface flatness, electron confinement, excess electrons, and band gap. Journal of Chemical Physics, 2003, 118, 4198-4205.	1.2	257
120	The interaction of oxygen with small gold clusters. Journal of Chemical Physics, 2003, 119, 2531-2537.	1.2	118
121	Effects of morphology on the electronic and transport properties of Sn-based clathrates. Journal of Chemical Physics, 2002, 117, 1302-1312.	1.2	34
122	Nonstoichiometry and chemical purity effects in thermoelectric Ba8Ga16Ge30 clathrate. Journal of Applied Physics, 2002, 92, 7281-7290.	1.1	60
123	How the folding rate constant of simple, single-domain proteins depends on the number of native contacts. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 3535-3539.	3.3	137
124	A model for the kinetics of protein folding: Kinetic Monte Carlo simulations and analytical results. Journal of Chemical Physics, 2002, 116, 5205.	1.2	24
125	A polynomial expansion of the quantum propagator, the Greenâ€™s function, and the spectral density operator. Journal of Chemical Physics, 2002, 116, 60.	1.2	19
126	The adsorption of molecular oxygen on neutral and negative Aun clusters (n=2â€“5). Chemical Physics Letters, 2002, 359, 493-499.	1.2	202

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127	Structure of the (001) surface of Î³ alumina. Journal of Chemical Physics, 2002, 117, 4509-4516.	1.2	31
128	Band structures and thermoelectric properties of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. Journal of Chemical Physics, 2001, 115, 8060-8073.	1.2	134
129	Structure and stability of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. Journal of Chemical Physics, 2001, 114, 10063-10074.	1.2	136
130	Control, with a rf field, of photon emission times by a single molecule and its connection to laser-induced localization of an electron in a double well. Journal of Chemical Physics, 2001, 115, 5989-5993.	1.2	32
131	Kinetic Monte Carlo simulation of titin unfolding. Journal of Chemical Physics, 2001, 114, 9663-9673.	1.2	61
132	Why are Clathrates Good Candidates for Thermoelectric Materials?. Journal of Solid State Chemistry, 2000, 149, 455-458.	1.4	129
133	Gallium Antimonide-Doped Germanium Clathrateâ€"A p-Type Thermoelectric Cage Structure. Journal of Solid State Chemistry, 2000, 151, 61-64.	1.4	40
134	Cation-vacancy ordering in dehydrated Na6[AlSiO4]6. Journal of Chemical Physics, 2000, 113, 10215-10225.	1.2	14
135	Nucleation and coarsening during epitaxy on a substrate subject to periodic strain: Spatial ordering and size uniformity. Journal of Chemical Physics, 2000, 113, 10323-10332.	1.2	9
136	Using Genetic Programming To Solve the SchrÃ¶dinger Equation. Journal of Physical Chemistry A, 2000, 104, 8540-8545.	1.1	22
137	Stochastic SchrÃ¶dinger equation. II. A study of the coherence seen in pump-probe experiments that use a strong pump laser. Journal of Chemical Physics, 1999, 111, 10137-10147.	1.2	6
138	The importance of self-interaction and nonlocal exchange corrections to the density functional theory of intracavity electrons in Na-doped sodalites. Journal of Chemical Physics, 1999, 110, 7457-7466.	1.2	11
139	Simulations of mobility and evaporation rate of adsorbate islands on solid surfaces. Journal of Chemical Physics, 1999, 111, 8639-8650.	1.2	26
140	Quantum dynamics with dissipation: A treatment of dephasing in the stochastic SchrÃ¶dinger equation. Journal of Chemical Physics, 1999, 111, 10126-10136.	1.2	35
141	Kinetic Monte Carlo simulations of nucleation on a surface with periodic strain: Spatial ordering and island-size distribution. Applied Physics Letters, 1999, 75, 926-928.	1.5	31
142	A new method for simulating the late stages of island coarsening in thin film growth: The role of island diffusion and evaporation. Journal of Chemical Physics, 1999, 110, 12151-12160.	1.2	27
143	Why clathrates are good thermoelectrics: A theoretical study of Sr8Ga16Ge30. Journal of Chemical Physics, 1999, 111, 3133-3144.	1.2	123
144	ELECTRONS SOLVATED IN ZEOLITES. , 1999, , .		1

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145	Island migration caused by the motion of the atoms at the border: Size and temperature dependence of the diffusion coefficient. Physical Review B, 1998, 57, R9459-R9462.	1.1	70
146	A kinetic model for island shape variations under epitaxial growth conditions. Surface Science, 1998, 405, L497-L502.	0.8	2
147	Ab-Initio-Based Transferable Potential for Sodalites. Journal of Physical Chemistry B, 1998, 102, 67-74.	1.2	22
148	Fitting potential-energy surfaces: A search in the function space by directed genetic programming. Journal of Chemical Physics, 1998, 108, 590-598.	1.2	50
149	Migration of hydrogen on a solid surface: the physics of the process and the methodology. , 1998, , .		0
150	The rate of photon absorption. , 1998, , .		0
151	Self-interaction-corrected band structure calculations for intracavity electrons in electro-sodalite. Journal of Chemical Physics, 1998, 109, 9977-9986.	1.2	17
152	Quantum-Size Effects on the Pattern Formation of Monatomic-Layer-High Metal Islands on Surfaces. Physical Review Letters, 1998, 80, 1026-1029.	2.9	18
153	Room-temperature fluorescence characteristics of single dye molecules adsorbed on a glass surface. Journal of Chemical Physics, 1998, 109, 7474-7485.	1.2	125
154	Some constraints involving the statistical properties of trajectories run in the Monte Carlo computation of a rate constant and their use in improving and testing the quality of sampling. Journal of Chemical Physics, 1998, 108, 8155-8160.	1.2	1
155	The reaction rate constant in a system with localized trajectories in the transition region: Classical and quantum dynamics. Journal of Chemical Physics, 1997, 107, 7787-7799.	1.2	13
156	The evaporation rate of a one-atom-high island on a solid surface: a thermodynamic theory of the size dependence. Surface Science, 1997, 373, L357-L362.	0.8	19
157	The effect of island coalescence on island density during epitaxial growth. Surface Science, 1997, 392, L56-L62.	0.8	21
158	Inter-layer diffusion and motion of adatoms in the vicinity of steps. Surface Science, 1996, 359, 245-252.	0.8	13
159	An effective medium theory study of Au islands on the Au(100) surface: reconstruction, adatom diffusion, and island formation. Surface Science, 1996, 365, 87-95.	0.8	14
160	Evaporation of single atoms from an adsorbate island or a step to a terrace: Evaporation rate and the underlying atomic-level mechanism. Physical Review B, 1996, 53, 16041-16049.	1.1	15
161	Multiple Time Scale Quantum Wavepacket Propagation:Â Electronâ^'Nuclear Dynamics. The Journal of Physical Chemistry, 1996, 100, 7867-7872.	2.9	58
162	An investigation of the electronic and optical properties of dehydrated sodalite fully doped with Na. Journal of Chemical Physics, 1996, 104, 8721-8729.	1.2	29

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163	Localization and delocalization of an electron in biased and unbiased quantum wells driven by a mono- and bichromatic laser field. Physical Review B, 1996, 53, 4657-4663.	1.1	16
164	The kinetics of H2dissociative chemisorption: The role of transients. Journal of Chemical Physics, 1995, 102, 8643-8655.	1.2	10
165	Evolution to equilibrium of the shape of an island formed by the aggregation of adsorbed atoms. Physical Review B, 1995, 51, 7827-7833.	1.1	22
166	Nonadiabatic effects on the charge transfer rate constant: A numerical study of a simple model system. Journal of Chemical Physics, 1995, 102, 9285-9295.	1.2	129
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