Horia Metiu

List of Publications by Year in Descending Order

333 papers	15,529 citations	65 h-index	105 g-index
343 ext. papers	16,377 ext. citations	4.5 avg, IF	6.68 L-index

#	Paper	IF	Citations
333	Properties of Methane and Carbon Adsorbed at the Interface between Molten NaBr and Ni(111). *Journal of Physical Chemistry C*, **2021**, 125, 3980-3987	3.8	3
332	Initial Steps in CH4 Pyrolysis on Cu and Ni. *Journal of Physical Chemistry C*, **2021**, 125, 18665-18672	3.8	1
331	Catalytic Methane Pyrolysis in Molten Alkali Chloride Salts Containing Iron. *ACS Catalysis*, **2020**, 10, 7032-7042	13.1	17
330	High-temperature heterogeneous catalysis in platinum nanoparticle molten salt suspensions. *Catalysis Science and Technology*, **2020**, 10, 625-629	5.5	2
329	Dry reforming of methane catalysed by molten metal alloys. *Nature Catalysis*, **2020**, 3, 83-89	36.5	57
328	Oxide Catalysts **2020**, 1343-1354		1
327	Catalytic Methane Pyrolysis with Liquid and Vapor Phase Tellurium. *ACS Catalysis*, **2020**, 10, 8223-8230	13.1	11
326	CO2-Free Hydrogen Production by Catalytic Pyrolysis of Hydrocarbon Feedstocks in Molten NiBi. *Energy & Fuels*, **2020**, 34, 16073-16080	4.1	8
325	Molecular Oxygen Activation on Suspended Doped Cerium(IV) Oxide Particles in Molten Chloride Salts. *Catalysis Letters*, **2020**, 150, 273-280	2.8	1
324	Properties of Negatively Charged Ruthenium Clusters in Molten Sodium Chloride. *Journal of Physical Chemistry C*, **2019**, 123, 16179-16185	3.8	5
323	Catalytic methane pyrolysis in molten MnCl2-KCl. *Applied Catalysis B: Environmental*, **2019**, 254, 659-666	21.8	42
322	Solid carbon production and recovery from high temperature methane pyrolysis in bubble columns containing molten metals and molten salts. *Carbon*, **2019**, 151, 181-191	10.4	35
321	Bromine and iodine for selective partial oxidation of propane and methane. *Applied Catalysis A: General*, **2019**, 580, 102-110	5.1	4
320	Rates of adsorption and desorption: Entropic contributions and errors due to mean-field approximations. *Journal of Chemical Physics*, **2019**, 150, 184702	3.9	2
319	Methane Pyrolysis with a Molten CuBi Alloy Catalyst. *ACS Catalysis*, **2019**, 9, 8337-8345	13.1	46
318	Oxide Catalysts **2018**, 1-12		
317	Chemistry of Solvated Electrons in Molten Alkali Chloride Salts. *Journal of Physical Chemistry C*, **2018**, 122, 19603-19612	3.8	7

316	THE ROLE OF COMPUTATIONS IN CATALYSIS. *Reviews in Computational Chemistry*, **2018**, 171-198		1
315	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	8.3	3
314	Chlorine Production by HCl Oxidation in a Molten Chloride Salt Catalyst. *Industrial & Engineering Chemistry Research*, **2018**, 57, 7795-7801	3.9	3
313	Molten salt chemical looping for reactive separation of HBr in a halogen-based natural gas conversion process. *Chemical Engineering Science*, **2017**, 160, 245-253	4.4	11
312	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	3.8	9
311	Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon. *Science*, **2017**, 358, 917-921	33.3	155
310	Oxygen Vacancy Formation on MoO3 Slabs and Ribbons. *Journal of Physical Chemistry C*, **2016**, 120, 19252-19264	3.8	25
309	Doped rhodium sulfide and thiospinels hydrogen evolution and oxidation electrocatalysts in strong acid electrolytes. *Journal of Applied Electrochemistry*, **2016**, 46, 497-503	2.6	10
308	Interaction between Monomeric Vanadium Oxide Clusters Supported on Titania and Its Influence on Their Reactivity. *Journal of Physical Chemistry C*, **2016**, 120, 13610-13621	3.8	8
307	Energy of Oxygen-Vacancy Formation on Oxide Surfaces: Role of the Spatial Distribution. *Journal of Physical Chemistry C*, **2016**, 120, 2320-2323	3.8	13
306	Structure of V2O5 hH2O Xerogels. *Journal of Physical Chemistry C*, **2016**, 120, 3986-3992	3.8	54
305	Halogen-Mediated Oxidative Dehydrogenation of Propane Using Iodine or Molten Lithium Iodide. *Catalysis Letters*, **2016**, 146, 744-754	2.8	7
304	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	3.8	4
303	Structure and Oxidizing Power of Single Layer V2O5. *Topics in Catalysis*, **2016**, 59, 809-816	2.3	5
302	Partial oxidation of propane with CO2 on Ru doped catalysts. *Catalysis Science and Technology*, **2016**, 6, 5483-5493	5.5	13
301	Reconstruction of Low-Index V2O5 Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 10500-10506	3.8	11
300	Hydrogen Abstraction Energies and Ammonia Binding to BEA, ZSM-5, and Quartz Doped with Al, Sc, B, or Ga. *Journal of Physical Chemistry C*, **2015**, 119, 16106-16114	3.8	7
299	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	3.8	17

298	CO2 methanation by Ru-doped ceria: the role of the oxidation state of the surface. *Catalysis Science and Technology*, **2015**, 5, 1783-1791	5.5	85
297	Hydrogen Dissociative Adsorption on Lanthana: Polaron Formation and the Role of AcidBase Interactions. *Journal of Physical Chemistry C*, **2015**, 119, 19876-19882	3.8	17
296	Catechol and HCl Adsorption on TiO2(110) in Vacuum and at the Water-TiO2 Interface. *Journal of Physical Chemistry Letters*, **2015**, 6, 2277-81	6.4	25
295	Stable electrocatalysts for autonomous photoelectrolysis of hydrobromic acid using single-junction solar cells. *Energy and Environmental Science*, **2014**, 7, 978-981	35.4	15
294	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, 8309-13	2.8	19
293	Investigation of the Electrocatalytic Activity of Rhodium Sulfide for Hydrogen Evolution and Hydrogen Oxidation. *Electrochimica Acta*, **2014**, 145, 224-230	6.7	20
292	Investigation of the active sites of rhodium sulfide for hydrogen evolution/oxidation using carbon monoxide as a probe. *Langmuir*, **2014**, 30, 5662-8	4	6
291	Oxygen Adsorption on Irreducible Oxides Doped with Higher Valence Ions: O2 Binding to the Dopant. *Journal of Physical Chemistry C*, **2014**, 118, 23070-23082	3.8	4
290	Catalytic Dry Reforming of Methane on Ruthenium-Doped Ceria and Ruthenium Supported on Ceria. *Topics in Catalysis*, **2014**, 57, 118-124	2.3	31
289	AcidBase Interaction and Its Role in Alkane Dissociative Chemisorption on Oxide Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 27336-27342	3.8	46
288	Ethane Activation by Nb-Doped NiO. *Journal of Physical Chemistry C*, **2013**, 117, 23597-23608	3.8	19
287	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	2.8	31
286	The Selective High-Yield Conversion of Methane Using Iodine-Catalyzed Methane Bromination. *ACS Catalysis*, **2013**, 3, 474-477	13.1	23
285	Catalysis by doped oxides. *Chemical Reviews*, **2013**, 113, 4391-427	68.1	565
284	Transition metal sulfide hydrogen evolution catalysts for hydrobromic acid electrolysis. *Langmuir*, **2013**, 29, 480-92	4	75
283	Interplay Between Bromine and Iodine in Oxidative Dehydrogenation. *ChemCatChem*, **2013**, 5, 1906-1910	3.2	18
282	Methane Dissociation on Li-, Na-, K-, and Cu-Doped Flat and Stepped CaO(001). *Journal of Physical Chemistry C*, **2013**, 117, 7114-7122	3.8	21
281	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	3.8	7

280	Gas-Phase Chemistry to Understand Electrochemical Hydrogen Evolution and Oxidation on Doped Transition Metal Sulfides. *Journal of the Electrochemical Society*, **2013**, 160, A1902-A1906	3.9	5
279	Hydrodebromination and Oligomerization of Dibromomethane. *ACS Catalysis*, **2012**, 2, 479-486	13.1	25
278	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	3.8	19
277	Halogen Adsorption on CeO2: The Role of Lewis AcidBase Pairing. *Journal of Physical Chemistry C*, **2012**, 116, 6664-6671	3.8	40
276	DFT Study of the Electronic Properties of LaOCl Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 681-691	3.8	13
275	Chemistry of Lewis AcidBase Pairs on Oxide Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 10439-10450	3.8	235
274	Preface: Special Topic Section on Photochemistry at Surfaces. *Journal of Chemical Physics*, **2012**, 137, 091501	3.9	
273	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	3.8	102
272	CH Bond Activation by Pd-substituted CeO2: Substituted Ions versus Reduced Species. *Chemistry of Materials*, **2011**, 23, 5432-5439	9.6	31
271	Choice of U for DFT+U Calculations for Titanium Oxides. *Journal of Physical Chemistry C*, **2011**, 115, 5841-5845	3.8	224
270	Chemistry of Doped Oxides: The Activation of Surface Oxygen and the Chemical Compensation Effect. *Journal of Physical Chemistry C*, **2011**, 115, 3065-3074	3.8	90
269	CO2 methanation on Ru-doped ceria. *Journal of Catalysis*, **2011**, 278, 297-309	7.3	292
268	Electronic Structure of Partially Reduced Rutile TiO2(110) Surface: Where Are the Unpaired Electrons Located?. *Journal of Physical Chemistry C*, **2011**, 115, 4696-4705	3.8	135
267	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution. *ChemCatChem*, **2011**, 3, 1607-1611	5.2	146
266	Dissociation of Methane on La2O3 Surfaces Doped with Cu, Mg, or Zn. *Journal of Physical Chemistry C*, **2011**, 115, 18239-18246	3.8	29
265	STM characterization of size-selected V1, V2, VO, and VO2 clusters on a TiO2(110)-(1 1) surface at room temperature. *Surface Science*, **2011**, 605, 972-976	1.8	27
264	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	3.8	29
263	DFT Studies of Oxygen Vacancies on Undoped and Doped La2O3 Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 12234-12244	3.8	86

262	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	3.8	38
261	Methane complete and partial oxidation catalyzed by Pt-doped CeO2. *Journal of Catalysis*, **2010**, 273, 125-137	7.3	163
260	CO oxidation by Ti- and Al-doped ZnO: Oxygen activation by adsorption on the dopant. *Journal of Catalysis*, **2009**, 266, 50-58	7.3	53
259	Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. *Surface Science*, **2009**, 603, 1724-1730	1.8	86
258	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	3.8	36
257	Selective promotion of different modes of methanol adsorption via the cation substitutional doping of a ZnO(101□0) surface. *Journal of Catalysis*, **2008**, 254, 325-331	7.3	33
256	O2 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	3.9	95
255	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	3.9	52
254	CO Oxidation by Rutile TiO2(110) Doped with V, W, Cr, Mo, and Mn. *Journal of Physical Chemistry C*, **2008**, 112, 12398-12408	3.8	108
253	Inelastic scattering with Chebyshev polynomials and preconditioned conjugate gradient minimization. *Journal of Physical Chemistry A*, **2008**, 112, 2728-37	2.8	
252	Preface to special topic: a survey of some new developments in heterogeneous catalysis. *Journal of Chemical Physics*, **2008**, 128, 182501	3.9	17
251	Size and pressure independent kinetics of CO oxidation on alumina-supported iridium nanoparticles. *International Journal of Chemical Kinetics*, **2008**, 40, 826-830	1.4	4
250	Vacancy formation and CO adsorption on gold-doped ceria surfaces. *Surface Science*, **2008**, 602, 2734-2742	1.8	115
249	Nanoscale current imaging of the conducting channels in proton exchange membrane fuel cells. *Nano Letters*, **2007**, 7, 227-32	11.5	77
248	Modification of the Oxidative Power of ZnO(101 0) Surface by Substituting Some Surface Zn Atoms with Other Metals. *Journal of Physical Chemistry C*, **2007**, 111, 8617-8622	3.8	57
247	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	3.8	27
246	Segregation at the surface of an Au/Pd alloy exposed to CO. *Surface Science*, **2007**, 601, 5332-5339	1.8	82
245	Catalysis by doped oxides: CO oxidation by AuxCe1□O2. *Journal of Catalysis*, **2007**, 245, 205-214	7.3	298

244	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. *Journal of Chemical Physics*, **2007**, 126, 204711	3.9	108
243	Density functional study of the interaction between small Au clusters, Au(n) (n=1-7) and the rutile TiO2 surface. II. Adsorption on a partially reduced surface. *Journal of Chemical Physics*, **2007**, 127, 244708	3.9	48
242	Density functional study of the charge on Aun clusters (n=1-7) supported on a partially reduced rutile TiO2(110): are all clusters negatively charged?. *Journal of Chemical Physics*, **2007**, 126, 104701	3.9	65
241	Catalysis by very small Au clusters. *Current Opinion in Solid State and Materials Science*, **2007**, 11, 62-75	12	107
240	VOx(x= 1-2) Submonolayers Supported on Rutile TiO2(110) and CeO2(111) Surfaces: 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	3.8	42
239	Dynamics of H2O and Na+ in nafion membranes. *Journal of Physical Chemistry B*, **2007**, 111, 2490-4	3.4	47
238	Efficient electrocatalyst utilization: electrochemical deposition of Pt nanoparticles using nafion membrane as a template. *Journal of Physical Chemistry B*, **2006**, 110, 7119-21	3.4	18
237	Minimum-error method for scattering problems in quantum mechanics: Two stable and efficient implementations. *Journal of Physical Chemistry A*, **2006**, 110, 10513-20	2.8	3
236	Pinning mononuclear Au on the surface of titania. *Journal of Physical Chemistry B*, **2006**, 110, 663-6	3.4	22
235	Formation, deposition and examination of size selected metal clusters on semiconductor surfaces: An experimental setup. *International Journal of Mass Spectrometry*, **2006**, 254, 202-209	1.9	29
234	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	2.8	100
233	Pinning mass-selected Agn clusters on the TiO2(110)-1x1 surface via deposition at high kinetic energy. *Journal of Chemical Physics*, **2005**, 123, 204701	3.9	26
232	Landing of size-selected Agn+ clusters on single crystal TiO2 (110)-(1x1) surfaces at room temperature. *Journal of Chemical Physics*, **2005**, 122, 81102	3.9	56
231	Structure of hydrated Na-Nafion polymer membranes. *Journal of Physical Chemistry B*, **2005**, 109, 24244-53	3.4	62
230	Electrolithographic investigations of the hydrophilic channels in Nafion membranes. *Journal of Physical Chemistry B*, **2005**, 109, 3252-6	3.4	31
229	Where does the planar-to-nonplanar turnover occur in small gold clusters?. *Journal of the American Chemical Society*, **2005**, 127, 1049-52	16.4	198
228	Excess proton solvation and delocalization in a hydrophilic pocket of the proton conducting polymer membrane nafion. *Journal of Physical Chemistry B*, **2005**, 109, 3727-30	3.4	118
227	Intact size-selected Au(n) clusters on a TiO2(110)-(1 x 1) surface at room temperature. *Journal of the American Chemical Society*, **2005**, 127, 13516-8	16.4	133

226	The nucleation sites of Ag clusters grown by vapor deposition on a TiO2(110)-1□ surface. *Surface Science*, **2005**, 575, 60-68	1.8	31
225	The binding of the noble metal cations Au+ and Ag+ to propene. *Chemical Physics Letters*, **2005**, 412, 416-419	2.5	8
224	Preface: Recent developments in density functional theory: Orbital dependent functionals. *Journal of Chemical Physics*, **2005**, 123, 062101	3.9	1
223	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, 7738-40	3.9	9
222	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, 3756-66	3.9	90
221	Density functional study of the adsorption of propene on silver clusters, Agmq (m=1□; q=0, +1). *Journal of Chemical Physics*, **2004**, 121, 9925-9930	3.9	37
220	A study of the reactions of molecular hydrogen with small gold clusters. *Journal of Chemical Physics* , **2004**, 120, 5169-75	3.9	90
219	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	3.9	56
218	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	2.5	14
217	Adsorption of gold on stoichiometric and reduced rutile TiO2 (110) surfaces. *Journal of Chemical Physics*, **2003**, 118, 6536-6551	3.9	186
216	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	3.9	240
215	The interaction of oxygen with small gold clusters. *Journal of Chemical Physics*, **2003**, 119, 2531-2537	3.9	113
214	The adsorption of molecular oxygen on neutral and negative Aun clusters (n=2□). *Chemical Physics Letters*, **2002**, 359, 493-499	2.5	190
213	Structure of the (001) surface of □alumina. *Journal of Chemical Physics*, **2002**, 117, 4509-4516	3.9	27
212	Effects of morphology on the electronic and transport properties of Sn-based clathrates. *Journal of Chemical Physics*, **2002**, 117, 1302-1312	3.9	32
211	Nonstoichiometry and chemical purity effects in thermoelectric Ba8Ga16Ge30 clathrate. *Journal of Applied Physics*, **2002**, 92, 7281-7290	2.5	58
210	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, 3535-9	11.5	127
209	A model for the kinetics of protein folding: Kinetic Monte Carlo simulations and analytical results. *Journal of Chemical Physics*, **2002**, 116, 5205	3.9	22

208	A polynomial expansion of the quantum propagator, the Green function, and the spectral density operator. *Journal of Chemical Physics*, **2002**, 116, 60	3.9	17
207	Band structures and thermoelectric properties of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. *Journal of Chemical Physics*, **2001**, 115, 8060-8073	3.9	128
206	Structure and stability of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. *Journal of Chemical Physics*, **2001**, 114, 10063-10074	3.9	126
205	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	3.9	32
204	Kinetic Monte Carlo simulation of titin unfolding. *Journal of Chemical Physics*, **2001**, 114, 9663-9673	3.9	57
203	Why are Clathrates Good Candidates for Thermoelectric Materials?. *Journal of Solid State Chemistry*, **2000**, 149, 455-458	3.3	117
202	Gallium Antimonide-Doped Germanium Clathrate: A p-Type Thermoelectric Cage Structure. *Journal of Solid State Chemistry*, **2000**, 151, 61-64	3.3	37
201	Cation-vacancy ordering in dehydrated Na6[AlSiO4]6. *Journal of Chemical Physics*, **2000**, 113, 10215-10225	3.9	14
200	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	3.9	9
199	Using Genetic Programming To Solve the Schrödinger Equation. *Journal of Physical Chemistry A*, **2000**, 104, 8540-8545	2.8	19
198	Stochastic Schrödinger 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	3.9	5
197	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	3.9	10
196	Simulations of mobility and evaporation rate of adsorbate islands on solid surfaces. *Journal of Chemical Physics*, **1999**, 111, 8639-8650	3.9	25
195	Quantum dynamics with dissipation: A treatment of dephasing in the stochastic Schrödinger equation. *Journal of Chemical Physics*, **1999**, 111, 10126-10136	3.9	32
194	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	3.4	30
193	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	3.9	26
192	Why clathrates are good thermoelectrics: A theoretical study of Sr8Ga16Ge30. *Journal of Chemical Physics*, **1999**, 111, 3133-3144	3.9	116
191	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	3.3	67

190	A kinetic model for island shape variations under epitaxial growth conditions. *Surface Science*, **1998**, 405, L497-L502	1.8	2
189	Ab-Initio-Based Transferable Potential for Sodalites. *Journal of Physical Chemistry B*, **1998**, 102, 67-74	3.4	21
188	Fitting potential-energy surfaces: A search in the function space by directed genetic programming. *Journal of Chemical Physics*, **1998**, 108, 590-598	3.9	48
187	Self-interaction-corrected band structure calculations for intracavity electrons in electro-sodalite. *Journal of Chemical Physics*, **1998**, 109, 9977-9986	3.9	16
186	Quantum-Size Effects on the Pattern Formation of Monatomic-Layer-High Metal Islands on Surfaces. *Physical Review Letters*, **1998**, 80, 1026-1029	7.4	18
185	Room-temperature fluorescence characteristics of single dye molecules adsorbed on a glass surface. *Journal of Chemical Physics*, **1998**, 109, 7474-7485	3.9	121
184	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	3.9	1
183	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	3.9	13
182	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	1.8	19
181	The effect of island coalescence on island density during epitaxial growth. *Surface Science*, **1997**, 392, L56-L62	1.8	20
180	Inter-layer diffusion and motion of adatoms in the vicinity of steps. *Surface Science*, **1996**, 359, 245-252	1.8	13
179	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	1.8	14
178	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	3.3	15
177	Multiple Time Scale Quantum Wavepacket Propagation: Electron Nuclear Dynamics. *The Journal of Physical Chemistry*, **1996**, 100, 7867-7872		49
176	An investigation of the electronic and optical properties of dehydrated sodalite fully doped with Na. *Journal of Chemical Physics*, **1996**, 104, 8721-8729	3.9	27
175	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	3.3	15
174	The kinetics of H2 dissociative chemisorption: The role of transients. *Journal of Chemical Physics*, **1995**, 102, 8643-8655	3.9	10
173	Evolution to equilibrium of the shape of an island formed by the aggregation of adsorbed atoms. *Physical Review B*, **1995**, 51, 7827-7833	3.3	20

172	Nonadiabatic effects on the charge transfer rate constant: A numerical study of a simple model system. *Journal of Chemical Physics*, **1995**, 102, 9285-9295	3.9	103
171	Submonolayer growth with repulsive impurities: Island density scaling with anomalous diffusion. *Physical Review Letters*, **1995**, 74, 4495-4498	7.4	47
170	Effect of small-cluster mobility and dissociation on the island density in epitaxial growth. *Physical Review B*, **1995**, 52, 2907-2913	3.3	52
169	Efficient absorption line shape calculations for an electron coupled to many quantum degrees of freedom: Applications to an electron solvated in dry sodalite and halo-sodalites. *Journal of Chemical Physics*, **1995**, 103, 4455-4465	3.9	8
168	Absolute negative resistance in double-barrier heterostructures in a strong laser field. *Physical Review B*, **1995**, 51, 4193-4199	3.3	40
167	Missing dimer vacancies ordering on the Si(100) surface. *Surface Science*, **1995**, 336, 303-313	1.8	29
166	The properties of electrons in sodalite saturated with alkali atoms. *Journal of Chemical Physics*, **1994**, 100, 6944-6952	3.9	24
165	Stability and kinetics of step motion on crystal surfaces. *Physical Review E*, **1994**, 49, 2601-2616	2.4	91
164	The mobility of Pt atoms and small Pt clusters on Pt(111) and its implications for the early stages of epitaxial growth. *Surface Science*, **1994**, 321, 161-171	1.8	49
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