Horia Metiu

List of Publications by Citations

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	Catalysis by doped oxides. *Chemical Reviews*, **2013**, 113, 4391-427	68.1	565
332	Catalysis by doped oxides: CO oxidation by AuxCe1−xO2. *Journal of Catalysis*, **2007**, 245, 205-214	7.3	298
331	CO2 methanation on Ru-doped ceria. *Journal of Catalysis*, **2011**, 278, 297-309	7.3	292
330	An efficient procedure for calculating the evolution of the wave function by fast Fourier transform methods for systems with spatially extended wave function and localized potential. *Journal of Chemical Physics*, **1987**, 86, 5009-5017	3.9	291
329	The interaction between electromagnetic resonances and its role in spectroscopic studies of molecules adsorbed on colloidal particles or metal spheres. *Surface Science*, **1981**, 110, 189-204	1.8	270
328	The effects of the interaction between resonances in the electromagnetic response of a sphere-plane structure; applications to surface enhanced spectroscopy. *Surface Science*, **1983**, 124, 506-528	1.8	252
327	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
326	Chemistry of Lewis Acid−Base Pairs on Oxide Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 10439-10450	4.8	235
325	Choice of U for DFT+U Calculations for Titanium Oxides. *Journal of Physical Chemistry C*, **2011**, 115, 5841-5845	4.8	224
324	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
323	The adsorption of molecular oxygen on neutral and negative Aun clusters (n=2−8). *Chemical Physics Letters*, **2002**, 359, 493-499	2.5	190
322	Adsorption of gold on stoichiometric and reduced rutile TiO2 (110) surfaces. *Journal of Chemical Physics*, **2003**, 118, 6536-6551	3.9	186
321	Methane complete and partial oxidation catalyzed by Pt-doped CeO2. *Journal of Catalysis*, **2010**, 273, 125-137	7.3	163
320	A strategy for time dependent quantum mechanical calculations using a Gaussian wave packet representation of the wave function. *Journal of Chemical Physics*, **1985**, 83, 3009-3027	3.9	163
319	Laser-induced localization of an electron in a double-well quantum structure. *Physical Review Letters*, **1992**, 69, 1986-1988	7.4	156
318	Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon. *Science*, **2017**, 358, 917-921	33.3	155
317	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution. *ChemCatChem*, **2011**, 3, 1607-1611	5.2	146

316	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
315	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
314	The evolution of the wave function in a curve crossing problem computed by a fast Fourier transform method. *Journal of Chemical Physics*, **1988**, 88, 4957-4966	3.9	133
313	A quantum mechanical study of predissociation dynamics of NaI excited by a femtosecond laser pulse. *Journal of Chemical Physics*, **1989**, 90, 6116-6128	3.9	132
312	A surface Penning ionization study of the CO/Ni(111) system. *Journal of Chemical Physics*, **1983**, 78, 4256-4269	3.9	130
311	Band structures and thermoelectric properties of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. *Journal of Chemical Physics*, **2001**, 115, 8060-8073	3.9	128
310	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
309	Hydrodynamic theory for vibrational relaxation in liquids. *Physical Review A*, **1977**, 15, 361-371	2.6	127
308	Classical theory of light scattering by an adsorbed molecule. I. Theory. *Journal of Chemical Physics*, **1979**, 70, 1602-1613	3.9	127
307	Structure and stability of the clathrates Ba8Ga16Ge30, Sr8Ga16Ge30, Ba8Ga16Si30, and Ba8In16Sn30. *Journal of Chemical Physics*, **2001**, 114, 10063-10074	3.9	126
306	Room-temperature fluorescence characteristics of single dye molecules adsorbed on a glass surface. *Journal of Chemical Physics*, **1998**, 109, 7474-7485	3.9	121
305	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
304	Why are Clathrates Good Candidates for Thermoelectric Materials?. *Journal of Solid State Chemistry*, **2000**, 149, 455-458	3.3	117
303	Why clathrates are good thermoelectrics: A theoretical study of Sr8Ga16Ge30. *Journal of Chemical Physics*, **1999**, 111, 3133-3144	3.9	116
302	Molecular state evolution after excitation with an ultra-short laser pulse: A quantum analysis of NaI and NaBr dissociation. *Chemical Physics Letters*, **1988**, 152, 1-7	2.5	116
301	Vacancy formation and CO adsorption on gold-doped ceria surfaces. *Surface Science*, **2008**, 602, 2734-2742	1.8	115
300	The interaction of oxygen with small gold clusters. *Journal of Chemical Physics*, **2003**, 119, 2531-2537	3.9	113
299	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

298	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. *Journal of Chemical Physics*, **2007**, 126, 204711	3.9	108
297	Catalysis by very small Au clusters. *Current Opinion in Solid State and Materials Science*, **2007**, 11, 62-75	12	107
296	The dynamics of H2 dissociation on Ni(100): A quantum mechanical study of a restricted two-dimensional model. *Journal of Chemical Physics*, **1987**, 86, 1026-1035	3.9	107
295	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
294	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
293	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
292	Properties of an electron in a quantum double well driven by a strong laser: Localization, low-frequency, and even-harmonic generation. *Physical Review A*, **1993**, 47, 3299-3310	2.6	100
291	Dynamics of phase separation of crystal surfaces. *Physical Review B*, **1993**, 48, 5808-5817	3.3	100
290	Stochastic theory of the kinetics of phase transitions. *Journal of Chemical Physics*, **1976**, 64, 292-299	3.9	96
289	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
288	Theory of rate processes at metal surfaces. II. The role of substrate electronic excitations. *Journal of Chemical Physics*, **1981**, 74, 2641-2653	3.9	94
287	Kinetic mechanism for island shape variations caused by changes in the growth temperature. *Physical Review Letters*, **1993**, 71, 2967-2970	7.4	91
286	Stability and kinetics of step motion on crystal surfaces. *Physical Review E*, **1994**, 49, 2601-2616	2.4	91
285	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
284	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
283	A study of the reactions of molecular hydrogen with small gold clusters. *Journal of Chemical Physics* , **2004**, 120, 5169-75	3.9	90
282	DFT Studies of Oxygen Vacancies on Undoped and Doped La2O3 Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 12234-12244	3.8	86
281	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

280	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
279	Detection by Metastable Quenching Spectroscopy of Enhanced Back-Donation from a Ni(111) Surface to the 2□ Orbital of Chemisorbed CO, Caused by Coadsorption of Potassium. *Physical Review Letters*, **1983**, 51, 1803-1806	7.4	85
278	Segregation at the surface of an Au/Pd alloy exposed to CO. *Surface Science*, **2007**, 601, 5332-5339	1.8	82
277	A one-dimensional microscopic quantum mechanical theory of light enhanced desorption. *Surface Science*, **1981**, 109, 191-206	1.8	81
276	Nanoscale current imaging of the conducting channels in proton exchange membrane fuel cells. *Nano Letters*, **2007**, 7, 227-32	11.5	77
275	Light scattering by a molecule near a solid surface. II. Model calculations. *Journal of Chemical Physics*, **1979**, 70, 2297-2309	3.9	77
274	Unusual metastable-quenching spectrum of K/Ni(111) and its explanation by a new quenching mechanism. *Physical Review Letters*, **1985**, 54, 1440-1443	7.4	76
273	Transition metal sulfide hydrogen evolution catalysts for hydrobromic acid electrolysis. *Langmuir*, **2013**, 29, 480-92	4	75
272	Mean-trajectory approximation for charge- and energy-transfer processes at surfaces. *Physical Review B*, **1985**, 32, 851-867	3.3	75
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270	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
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268	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
267	Classical theory of light scattering by a molecule located near a solid surface. *Chemical Physics Letters*, **1978**, 60, 59-64	2.5	64
266	Two-photon excitation of NaI with femtosecond laser pulses. *Journal of Chemical Physics*, **1989**, 91, 1596-1602	3.9	63
265	Structure of hydrated Na-Nafion polymer membranes. *Journal of Physical Chemistry B*, **2005**, 109, 24244-53	3.4	62
264	A time-dependent interpretation of the absorption spectrum of CH3ONO. *Journal of Chemical Physics*, **1990**, 92, 1-13	3.9	62
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262	Surface roughness in thin-film growth: The effect of mass transport between layers. *Physical Review B*, **1993**, 48, 4972-4975	3.3	60
261	Molecular dynamics simulations of energy flow at a solid surface. New methods using a small number of atoms. *Journal of Chemical Physics*, **1989**, 90, 1229-1236	3.9	60
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259	The enhancement of raman and fluorescent intensity by small surface roughness. changes in dipole emission. *Chemical Physics Letters*, **1980**, 74, 301-305	2.5	59
258	Electrodynamics at metal surfaces. IV. The electric fields caused by the polarization of a metal surface by an oscillating dipole. *Journal of Chemical Physics*, **1982**, 76, 1564-1573	3.9	59
257	Rotational mechanism for vibrational relaxation in rigid media. *Chemical Physics Letters*, **1977**, 48, 262-266	2.5	59
256	Nonstoichiometry and chemical purity effects in thermoelectric Ba8Ga16Ge30 clathrate. *Journal of Applied Physics*, **2002**, 92, 7281-7290	2.5	58
255	Dry reforming of methane catalysed by molten metal alloys. *Nature Catalysis*, **2020**, 3, 83-89	36.5	57
254	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
253	Kinetic Monte Carlo simulation of titin unfolding. *Journal of Chemical Physics*, **2001**, 114, 9663-9673	3.9	57
252	Multiphoton dissociation of a diatomic molecule: Laser intensity, frequency, and pulse shape dependence of the fragment momentum distribution. *Journal of Chemical Physics*, **1988**, 88, 5496-5505	3.9	57
251	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
250	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
249	A Gaussian wave packet method for studying time dependent quantum mechanics in a curve crossing system: Low energy motion, tunneling, and thermal dissipation. *Journal of Chemical Physics* , **1986**, 84, 6293-6311	3.9	56
248	Structure of V2O5□hH2O Xerogels. *Journal of Physical Chemistry C*, **2016**, 120, 3986-3992	3.8	54
247	Electrodynamics at a metal surface with applications to the spectroscopy of adsorbed molecules. I. General theory. *Physical Review B*, **1980**, 22, 4731-4738	3.3	54
246	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
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243	Effect of small-cluster mobility and dissociation on the island density in epitaxial growth. *Physical Review B*, **1995**, 52, 2907-2913	3.3	52
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241	Exact classical simulation of hydrogen migration on Ni(100): The role of fluctuations, recrossing, and multiple jumps. *Journal of Chemical Physics*, **1990**, 93, 3614-3634	3.9	51
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239	A numerical study of the multiple Gaussian representation of time dependent wave functions of a Morse oscillator. *Journal of Chemical Physics*, **1986**, 84, 3250-3259	3.9	51
238	Multiple Time Scale Quantum Wavepacket Propagation: Electron□Nuclear Dynamics. *The Journal of Physical Chemistry*, **1996**, 100, 7867-7872		49
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233	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
232	A theoretical study of I2 vibrational motion after excitation with an ultrashort pulse. *Journal of Chemical Physics*, **1990**, 93, 5693-5699	3.9	48
231	Dynamics of H2O and Na+ in nafion membranes. *Journal of Physical Chemistry B*, **2007**, 111, 2490-4	3.4	47
230	Submonolayer growth with repulsive impurities: Island density scaling with anomalous diffusion. *Physical Review Letters*, **1995**, 74, 4495-4498	7.4	47
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227	Methane Pyrolysis with a Molten Cu□i Alloy Catalyst. *ACS Catalysis*, **2019**, 9, 8337-8345	13.1	46

226	Acid–Base Interaction and Its Role in Alkane Dissociative Chemisorption on Oxide Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 27336-27342	3.8	46
225	Luminescence and nonradiative energy transfer to surfaces. *Physical Review B*, **1980**, 21, 5565-5571	3.3	46
224	A test of the possibility of calculating absorption spectra by mixed quantum-classical methods. *Journal of Chemical Physics*, **1992**, 97, 4781-4791	3.9	45
223	Atomic Exchange between CO Molecules Coadsorbed with Potassium on Ni(111). *Physical Review Letters*, **1983**, 51, 1991-1994	7.4	45
222	Dynamical theory of migration of an adsorbed atom on solid surfaces. *Journal of Chemical Physics*, **1976**, 65, 2871-2882	3.9	45
221	Electron gas effects in the spectroscopy of molecules chemisorbed at a metal surface. I. Theory. *Journal of Chemical Physics*, **1980**, 72, 1996-2006	3.9	44
220	Numerical solution of the time-dependent Schrödinger equation in spherical coordinates by Fourier-transform methods. *Journal of Chemical Physics*, **1991**, 95, 7392-7400	3.9	43
219	Catalytic methane pyrolysis in molten MnCl2-KCl. *Applied Catalysis B: Environmental*, **2019**, 254, 659-666	21.8	42
218	VOx(x= 1–4) 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
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216	The fluorescence lifetime of a molecule emitting near a surface with small, random roughness. *Chemical Physics Letters*, **1982**, 85, 404-408	2.5	42
215	Hydrogen motion on a rigid Cu surface: The calculation of the site to site hopping rate by using flux–flux correlation functions. *Journal of Chemical Physics*, **1990**, 92, 2083-2098	3.9	41
214	Adsorption and diffusion sites of a Si atom on a reconstructed Si(100)-(2 × 1) surface. *Surface Science*, **1991**, 248, L250-L254	1.8	41
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209	Growth kinetics simulation of the Al-Ga self-organization on GaAs(100) stepped surfaces. *Surface Science*, **1991**, 245, 150-172	1.8	39

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207	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
206	Conditions leading to intense low-frequency generation and strong localization in two-level systems. *Physical Review A*, **1993**, 48, 2342-2345	2.6	38
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202	Density functional study of the adsorption of propene on silver clusters, Agmq (m=1–5; q=0, +1). *Journal of Chemical Physics*, **2004**, 121, 9925-9930	3.9	37
201	Gallium Antimonide-Doped Germanium Clathrate-I: A p-Type Thermoelectric Cage Structure. *Journal of Solid State Chemistry*, **2000**, 151, 61-64	3.3	37
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199	Study of adsorption and decomposition of NO on clean and oxygen-covered Ni(111) by metastable quenching spectroscopy. *Surface Science*, **1984**, 141, 591-603	1.8	37
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180	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
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176	Kinetic stability of missing-dimer and single-atom defects on Si(100). *Physical Review B*, **1993**, 48, 8166-8171	3.7	31
175	Angular resonances in the emission from a dipole located near a grating. *Surface Science*, **1981**, 109, 95-108	2.1	31
174	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
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169	Dissociation of Methane on La2O3 Surfaces Doped with Cu, Mg, or Zn. *Journal of Physical Chemistry C*, **2011**, 115, 18239-18246	3.8	29
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