Maite Alducin

List of Publications by Year in Descending Order

117 papers	2,390 citations	28 h-index	42 g-index
123 ext. papers	2,547 ext. citations	3.5 avg, IF	5.23 L-index

#	Paper	IF	Citations
117	Absence of isotope effects in the photo-induced desorption of CO from saturated Pd(111) at high laser fluence. *Chemical Physics*, **2022**, 558, 111518	2.3	1
116	O2 on Ag(110): A puzzle for exchange-correlation functionals. *Chemical Physics*, **2021**, 554, 111424	2.3	
115	High-Dimensional Atomistic Neural Network Potential to Study the Alignment-Resolved O Scattering from Highly Oriented Pyrolytic Graphite. *Journal of Physical Chemistry A*, **2021**, 125, 2588-2600	2.8	5
114	Insights into the Coadsorption and Reactivity of O and CO on Ru(0001) and Their Coverage Dependence. *Journal of Physical Chemistry C*, **2021**, 125, 12614-12627	3.8	1
113	Photoinduced Desorption Dynamics of CO from Pd(111): A Neural Network Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 4648-4659	6.4	8
112	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. *Applied Surface Science*, **2021**, 559, 149835	6.7	1
111	Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations. *Journal of Applied Physics*, **2020**, 127, 145102	2.5	4
110	Nonadiabatic Effects in Gas-Surface Dynamics. *Springer Handbooks*, **2020**, 929-965	1.3	
109	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. *Intermetallics*, **2019**, 106, 130-140	3.5	12
108	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. *Journal of Physical Chemistry C* , **2019**, 123, 15236-15243	3.8	7
107	CO Stretch Vibration Lives Long on Au(111). *Journal of Physical Chemistry Letters*, **2019**, 10, 1043-1047	6.4	14
106	Ab Initio Molecular Dynamics Study of Alignment-Resolved O2 Scattering from Highly Oriented Pyrolytic Graphite. *Journal of Physical Chemistry C*, **2019**, 123, 31094-31102	3.8	9
105	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). *Physical Review B*, **2019**, 100,	3.3	16
104	Vibrational response and motion of carbon monoxide on Cu(100) driven by femtosecond laser pulses: Molecular dynamics with electronic friction. *Physical Review B*, **2019**, 100,	3.3	10
103	Electrons and Phonons Cooperate in the Laser-Induced Desorption of CO from Pd(111). *Physical Review Letters*, **2019**, 123, 246802	7.4	10
102	Ultrafast Transient Dynamics of Adsorbates on Surfaces Deciphered: The Case of CO on Cu(100). *Physical Review Letters*, **2019**, 122, 016806	7.4	19
101	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 2287-2299	3.8	21

100	Electron-Mediated Phonon-Phonon Coupling Drives the Vibrational Relaxation of CO on Cu(100). *Physical Review Letters*, **2018**, 120, 156804	7.4	21
99	Ab initio molecular dynamics study of the Eley-Rideal reaction of H + Cl-Au(111) -rHCl + Au(111): Impact of energy dissipation to surface phonons and electron-hole pairs. *Journal of Chemical Physics*, **2018**, 148, 014702	3.9	22
98	Energy dissipation to tungsten surfaces upon hot-atom and Eley-Rideal recombination of H. *Physical Chemistry Chemical Physics*, **2018**, 20, 21334-21344	3.6	5
97	Communication: Fingerprints of reaction mechanisms in product distributions: Eley-Rideal-type reactions between D and CD/Cu(111). *Journal of Chemical Physics*, **2018**, 149, 031101	3.9	14
96	Electronic Stopping of Slow Protons in Transition and Rare Earth Metals: Breakdown of the Free Electron Gas Concept. *Physical Review Letters*, **2017**, 118, 103401	7.4	38
95	Vibrational Excitation of H Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. *Journal of Physical Chemistry C*, **2017**, 121, 13617-13633	3.8	22
94	Femtosecond laser induced desorption of H2,D2, and HD from Ru(0001): Dynamical promotion and suppression studied with ab initio molecular dynamics with electronic friction. *Physical Review B*, **2017**, 95,	3.3	22
93	Communication: Hot-atom abstraction dynamics of hydrogen from tungsten surfaces: The role of surface structure. *Journal of Chemical Physics*, **2017**, 147, 121103	3.9	10
92	Non-adiabatic effects in elementary reaction processes at metal surfaces. *Progress in Surface Science*, **2017**, 92, 317-340	6.6	62
91	Stereodynamics of Diatom Formation through Eley–Rideal Abstraction. *Journal of Physical Chemistry C*, **2017**, 121, 19849-19858	3.8	13
90	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. *Journal of Physical Chemistry C*, **2017**, 121, 20756-20762	3.8	8
89	Electronic Stopping of Slow Protons in Oxides: Scaling Properties. *Physical Review Letters*, **2017**, 119, 163401	7.4	24
88	Energy loss and surface temperature effects in ab initio molecular dynamics simulations: N adsorption on Ag(111) as a case study. *Physical Review B*, **2017**, 96,	3.3	16
87	Role of valence states of adsorbates in inelastic electron tunneling spectroscopy: A study of nitric oxide on Cu(110) and Cu(001). *Physical Review B*, **2016**, 94,	3.3	8
86	Molecular dynamics simulation of O adsorption on Ag(110) from first principles electronic structure calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 27366-27376	3.6	14
85	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). *Physical Review B*, **2016**, 93,	3.3	36
84	Surface electron density models for accurate ab initio molecular dynamics with electronic friction. *Physical Review B*, **2016**, 93,	3.3	50
83	Hydrogen abstraction from metal surfaces: when electron-hole pair excitations strongly affect hot-atom recombination. *Physical Chemistry Chemical Physics*, **2016**, 18, 31378-31383	3.6	27

82	Electron-Hole Pair Effects in Polyatomic Dissociative Chemisorption: Water on Ni(111). *Journal of Physical Chemistry Letters*, **2016**, 7, 327-31	6.4	64
81	Energy loss in gas-surface dynamics: Electron–hole pair and phonon excitation upon adsorbate relaxation. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 382, 26-31	1.2	16
80	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 382, 114-118	1.2	14
79	Modeling surface motion effects in N2 dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model. *Journal of Chemical Physics*, **2016**, 144, 244708	3.9	18
78	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). *Journal of Chemical Physics*, **2016**, 145, 044704	3.9	44
77	Effects of electronic relaxation processes on vibrational linewidths of adsorbates on surfaces: The case of CO/Cu(100). *Physical Review B*, **2016**, 94,	3.3	28
76	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. *Journal of Physical Chemistry C*, **2016**, 120, 17357-17364	3.8	32
75	Influence of the van der Waals interaction in the dissociation dynamics of N2 on W(110) from first principles. *Journal of Chemical Physics*, **2015**, 142, 074704	3.9	22
74	Energy Dissipation to Tungsten Surfaces upon Eley–Rideal Recombination of N2 and H2. *Journal of Physical Chemistry C*, **2015**, 119, 15434-15442	3.8	37
73	The dynamics of adsorption and dissociation of N2 in a monolayer of iron on W(110). *Physical Chemistry Chemical Physics*, **2015**, 17, 19432-45	3.6	7
72	Ab initio molecular dynamics with simultaneous electron and phonon excitations: Application to the relaxation of hot atoms and molecules on metal surfaces. *Physical Review B*, **2015**, 92,	3.3	69
71	Angular distributions and rovibrational excitation of N2 molecules recombined on N-covered Ag(111) by the Eley–Rideal mechanism. *Catalysis Today*, **2015**, 244, 115-121	5.3	5
70	Dissociative dynamics of O2 on Ag(110). *Physical Chemistry Chemical Physics*, **2015**, 17, 9436-45	3.6	21
69	Surface strain improves molecular adsorption but hampers dissociation for N2 on the Fe/W(110) surface. *Physical Review Letters*, **2014**, 113, 066103	7.4	27
68	Vibrational lifetimes of hydrogen on lead films: an ab initio molecular dynamics with electronic friction (AIMDEF) study. *Journal of Chemical Physics*, **2014**, 141, 234702	3.9	36
67	Role of physisorption states in molecular scattering: a semilocal density-functional theory study on O2/Ag(111). *Physical Review Letters*, **2014**, 112, 156101	7.4	27
66	Electronic friction dominates hydrogen hot-atom relaxation on Pd(100). *Physical Review Letters*, **2014**, 112, 103203	7.4	97
65	Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111). *Journal of Chemical Physics*, **2014**, 141, 054705	3.9	37

64	Adiabatic Energy Loss in Hyperthermal H Atom Collisions with Cu and Au: A Basis for Testing the Importance of Nonadiabatic Energy Loss. *Journal of Physical Chemistry Letters*, **2013**, 4, 3735-3740	6.4	42
63	Efficient N2 Formation on Ag(111) by Eley-Rideal Recombination of Hyperthermal Atoms. *Journal of Physical Chemistry Letters*, **2013**, 4, 3704-3709	6.4	30
62	Ready, Set and no Action: A Static Perspective on Potential Energy Surfaces commonly used in Gas-Surface Dynamics. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	14
61	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 9779-9790	3.8	20
60	Energy Dissipation Channels in Reactive and Non-reactive Scattering at Surfaces. *Springer Series in Surface Sciences*, **2013**, 371-388	0.4	5
59	Dissociative and non-dissociative adsorption dynamics of N2 on Fe(110). *Physical Chemistry Chemical Physics*, **2012**, 14, 7471-80	3.6	32
58	Dynamics of Nitrogen Scattering off N-Covered Ag(111). *Journal of Physical Chemistry C*, **2012**, 116, 21903-21912	3.8	13
57	Energy dissipation channels in the adsorption of N on Ag(111). *Computational and Theoretical Chemistry*, **2012**, 990, 126-131	2	27
56	Non-adiabatic effects during the dissociative adsorption of O2at Ag(111)? A first-principles divide and conquer study. *New Journal of Physics*, **2012**, 14, 013050	2.9	43
55	Vibrational deexcitation and rotational excitation of H2 and D2 scattered from Cu(111): adiabatic versus non-adiabatic dynamics. *Journal of Chemical Physics*, **2012**, 137, 064707	3.9	40
54	Publisher's Note: Competition between Electron and Phonon Excitations in the Scattering of Nitrogen Atoms and Molecules off Tungsten and Silver Metal Surfaces [Phys. Rev. Lett. 108, 096101 (2012)]. *Physical Review Letters*, **2012**, 108,	7.4	3
53	Diffusion of hydrogen in Pd assisted by inelastic ballistic hot electrons. *Physical Review Letters*, **2012**, 108, 115902	7.4	18
52	Competition between electron and phonon excitations in the scattering of nitrogen atoms and molecules off tungsten and silver metal surfaces. *Physical Review Letters*, **2012**, 108, 096101	7.4	76
51	Non-reactive scattering of N2 from the W(110) surface studied with different exchange-correlation functionals. *Physical Chemistry Chemical Physics*, **2011**, 13, 4357-64	3.6	20
50	Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy. *Physical Review Letters*, **2010**, 104, 136101	7.4	36
49	Role of molecular electronic structure in inelastic electron tunneling spectroscopy: O2 on Ag(110). *Physical Review B*, **2010**, 82,	3.3	22
48	Juaristi et al. Reply:. *Physical Review Letters*, **2009**, 102,	7.4	28
47	Dissipative effects in the dynamics of N(2) on tungsten surfaces. *Journal of Physics Condensed Matter*, **2009**, 21, 264007	1.8	30

46	Dissociative dynamics of spin-triplet and spin-singlet O2 on Ag(100). *Journal of Chemical Physics*, **2008**, 129, 224702	3.9	37
45	The role of exchange-correlation functionals in the potential energy surface and dynamics of N(2) dissociation on W surfaces. *Journal of Chemical Physics*, **2008**, 128, 154704	3.9	48
44	The role of an electronic surface state in the stopping power of a swift charged particle in front of a metal. *Journal of Physics Condensed Matter*, **2008**, 20, 304209	1.8	14
43	Role of electron-hole pair excitations in the dissociative adsorption of diatomic molecules on metal surfaces. *Physical Review Letters*, **2008**, 100, 116102	7.4	201
42	Dissociative adsorption of N2 on W(1 1 0): Theoretical study of the dependence on the incidence angle. *Surface Science*, **2007**, 601, 3726-3730	1.8	12
41	Dynamic screening and electron dynamics in low-dimensional metal systems. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 258, 72-78	1.2	8
40	Spin dependent screening and Auger neutralization of singly-charged noble gas ions in metals. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 256, 24-29	1.2	1
39	Two dimensional behaviour of friction at a metal surface with a surface state. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 256, 383-386	1.2	4
38	Spin-dependent electron excitation and emission in the neutralization of He+ ions at paramagnetic surfaces. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 256, 423-428	1.2	1
37	Interaction of slow multicharged ions with surfaces. *Radiation Physics and Chemistry*, **2007**, 76, 412-417	2.5	3
36	3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces. *Physical Review A*, **2007**, 76,	2.6	4
35	Spin Polarization of Electrons Emitted in the Neutralization of He+ Ions in Solids **2007**, 153-183		
34	Low sticking probability in the nonactivated dissociation of N2 molecules on W(110). *Journal of Chemical Physics*, **2006**, 125, 144705	3.9	42
33	Why N2 molecules with thermal energy abundantly dissociate on W(100) and not on W(110). *Physical Review Letters*, **2006**, 97, 056102	7.4	74
32	Influence of plasmon-assisted charge exchange processes on ion-induced electron emission from metals. *Vacuum*, **2006**, 80, 554-560	3.7	
31	Spin effects in the screening and Auger neutralization of He+ ions in a spin-polarized electron gas. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 230, 431-437	1.2	6
30	Spin dependence in the neutralization of He+ ions in metals: An analysis of different contributions. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 232, 8-15	1.2	5
29	Electron emission in the Auger neutralization of a spin-polarized He+ ion embedded in a free electron gas. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 232, 73-78	1.2	5

28	Vicinage effects in the energy loss of slow LiH molecules in metals. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 232, 178-183	1.2	1
27	Spin-dependent electron emission from metals in the neutralization of He+ ions. *Physical Review A*, **2005**, 72,	2.6	14
26	Band-structure-based collisional model for electronic excitations in ion-surface collisions. *Physical Review A*, **2005**, 72,	2.6	6
25	Spin-dependent screening and Auger neutralization of He+ ions in metals. *Physical Review A*, **2004**, 70,	2.6	27
24	Spin-polarized electron excitation during the neutralization of He+ ions in metals. *Journal of Electron Spectroscopy and Related Phenomena*, **2004**, 137-140, 401-405	1.7	12
23	Time-dependent screening in a two-dimensional electron gas. *Surface Science*, **2004**, 559, 233-240	1.8	9
22	Energy Loss in the Interaction of Atomic Particles with Solid Surfaces. *Advances in Quantum Chemistry*, **2004**, 223-245	1.4	4
21	The relaxation rate in hot-electron dynamics: beyond the first-order Born approximation in kinetic theory. *Journal of Physics Condensed Matter*, **2003**, 15, 7859-7865	1.8	4
20	Ion induced electronic excitations in a spin-polarized electron gas. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 203, 83-88	1.2	2
19	Time-dependent image potential at a metal surface. *Journal of Electron Spectroscopy and Related Phenomena*, **2003**, 129, 105-109	1.7	9
18	Relaxation rate of excited electrons in an electron gas. *Journal of Electron Spectroscopy and Related Phenomena*, **2003**, 129, 117-126	1.7	2
17	Spin□olarization effects in the interaction of light atoms with a free electron gas. *Journal of Electron Spectroscopy and Related Phenomena*, **2003**, 129, 207-211	1.7	3
16	Minimum dipole moment required to bind an electron to a screened dipole field. *Physical Review B*, **2003**, 67,	3.3	7
15	Energy loss of ions at metal surfaces: Band-structure effects. *Physical Review A*, **2003**, 67,	2.6	26
14	Role of the bound-state wave function in capture-loss rates: Slow proton in an electron gas. *Physical Review A*, **2003**, 68,	2.6	8
13	Effect of surface band structure in the energy loss of ions at surfaces. *Nuclear Instruments & Methods in Physics Research B*, **2002**, 193, 585-589	1.2	11
12	Nonlinear effects in the energy loss of a slow dipole in a free-electron gas. *Physical Review A*, **2002**, 66,	2.6	4
11	Relaxation of excited electrons in an electron gas: A mean-field approach with charge and spin polarizations. *Physical Review B*, **2002**, 65,	3.3	6

10	Dielectric response of covered metal surfaces: Oxidation of Al(111). *Physical Review B*, **2001**, 64,	3.3	6
9	Relaxation of excited electrons in a paramagnetic electron gas: The role of spins in screening and scattering. *Physical Review B*, **2001**, 64,	3.3	7
8	Surface photoelectric effect induced by small clusters impinging on solid surfaces. *Nuclear Instruments & Methods in Physics Research B*, **2000**, 164-165, 662-670	1.2	
7	Photon emission from Agn+ clusters: Role of the ionization potential. *Nuclear Instruments & Methods in Physics Research B*, **1997**, 125, 7-12	1.2	
6	Radiative neutralization of small clusters impinging on solid surfaces. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1997**, 41, 143-150		5
5	Auger deexcitation in a helium atom induced by a metal surface. *Physical Review A*, **1996**, 53, 4222-4227	2.6	18
4	Auger deexcitation rates in grazing atom-surface collisions. *Nuclear Instruments & Methods in Physics Research B*, **1995**, 98, 424-428	1.2	1
3	Local theory of Auger neutralization for slow and compact ions interacting with metal surfaces. *Physical Review A*, **1994**, 49, 4716-4725	2.6	49
2	Auger intra-atomic transitions in grazing atom-surface collisions. *Physical Review B*, **1994**, 49, 14589-14598	3.3	13
1	Auger capture rates for a slow ion close to a metal surface. *Nuclear Instruments & Methods in Physics Research B*, **1992**, 67, 157-159	1.2	20