

Maite Alducin

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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	Role of electron-hole pair excitations in the dissociative adsorption of diatomic molecules on metal surfaces. <i>Physical Review Letters</i> , 2008 , 100, 116102	7.4	201
116	Electronic friction dominates hydrogen hot-atom relaxation on Pd(100). <i>Physical Review Letters</i> , 2014 , 112, 103203	7.4	97
115	Competition between electron and phonon excitations in the scattering of nitrogen atoms and molecules off tungsten and silver metal surfaces. <i>Physical Review Letters</i> , 2012 , 108, 096101	7.4	76
114	Why N ₂ molecules with thermal energy abundantly dissociate on W(100) and not on W(110). <i>Physical Review Letters</i> , 2006 , 97, 056102	7.4	74
113	Ab initio molecular dynamics with simultaneous electron and phonon excitations: Application to the relaxation of hot atoms and molecules on metal surfaces. <i>Physical Review B</i> , 2015 , 92,	3.3	69
112	Electron-Hole Pair Effects in Polyatomic Dissociative Chemisorption: Water on Ni(111). <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 327-31	6.4	64
111	Non-adiabatic effects in elementary reaction processes at metal surfaces. <i>Progress in Surface Science</i> , 2017 , 92, 317-340	6.6	62
110	Surface electron density models for accurate ab initio molecular dynamics with electronic friction. <i>Physical Review B</i> , 2016 , 93,	3.3	50
109	Local theory of Auger neutralization for slow and compact ions interacting with metal surfaces. <i>Physical Review A</i> , 1994 , 49, 4716-4725	2.6	49
108	The role of exchange-correlation functionals in the potential energy surface and dynamics of N(2) dissociation on W surfaces. <i>Journal of Chemical Physics</i> , 2008 , 128, 154704	3.9	48
107	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). <i>Journal of Chemical Physics</i> , 2016 , 145, 044704	3.9	44
106	Non-adiabatic effects during the dissociative adsorption of O ₂ at Ag(111)? A first-principles divide and conquer study. <i>New Journal of Physics</i> , 2012 , 14, 013050	2.9	43
105	Adiabatic Energy Loss in Hyperthermal H Atom Collisions with Cu and Au: A Basis for Testing the Importance of Nonadiabatic Energy Loss. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3735-3740	6.4	42
104	Low sticking probability in the nonactivated dissociation of N ₂ molecules on W(110). <i>Journal of Chemical Physics</i> , 2006 , 125, 144705	3.9	42
103	Vibrational deexcitation and rotational excitation of H ₂ and D ₂ scattered from Cu(111): adiabatic versus non-adiabatic dynamics. <i>Journal of Chemical Physics</i> , 2012 , 137, 064707	3.9	40
102	Electronic Stopping of Slow Protons in Transition and Rare Earth Metals: Breakdown of the Free Electron Gas Concept. <i>Physical Review Letters</i> , 2017 , 118, 103401	7.4	38
101	Energy Dissipation to Tungsten Surfaces upon Eley-Rideal Recombination of N ₂ and H ₂ . <i>Journal of Physical Chemistry C</i> , 2015 , 119, 15434-15442	3.8	37

100	Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111). <i>Journal of Chemical Physics</i> , 2014 , 141, 054705	3.9	37
99	Dissociative dynamics of spin-triplet and spin-singlet O ₂ on Ag(100). <i>Journal of Chemical Physics</i> , 2008 , 129, 224702	3.9	37
98	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). <i>Physical Review B</i> , 2016 , 93,	3.3	36
97	Vibrational lifetimes of hydrogen on lead films: an ab initio molecular dynamics with electronic friction (AIMDEF) study. <i>Journal of Chemical Physics</i> , 2014 , 141, 234702	3.9	36
96	Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy. <i>Physical Review Letters</i> , 2010 , 104, 136101	7.4	36
95	Dissociative and non-dissociative adsorption dynamics of N ₂ on Fe(110). <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 7471-80	3.6	32
94	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 17357-17364	3.8	32
93	Efficient N ₂ Formation on Ag(111) by Eley-Rideal Recombination of Hyperthermal Atoms. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3704-3709	6.4	30
92	Dissipative effects in the dynamics of N(2) on tungsten surfaces. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 264007	1.8	30
91	Juaristi et al. Reply. <i>Physical Review Letters</i> , 2009 , 102,	7.4	28
90	Effects of electronic relaxation processes on vibrational linewidths of adsorbates on surfaces: The case of CO/Cu(100). <i>Physical Review B</i> , 2016 , 94,	3.3	28
89	Hydrogen abstraction from metal surfaces: when electron-hole pair excitations strongly affect hot-atom recombination. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 31378-31383	3.6	27
88	Surface strain improves molecular adsorption but hampers dissociation for N ₂ on the Fe/W(110) surface. <i>Physical Review Letters</i> , 2014 , 113, 066103	7.4	27
87	Role of physisorption states in molecular scattering: a semilocal density-functional theory study on O ₂ /Ag(111). <i>Physical Review Letters</i> , 2014 , 112, 156101	7.4	27
86	Energy dissipation channels in the adsorption of N on Ag(111). <i>Computational and Theoretical Chemistry</i> , 2012 , 990, 126-131	2	27
85	Spin-dependent screening and Auger neutralization of He ⁺ ions in metals. <i>Physical Review A</i> , 2004 , 70,	2.6	27
84	Energy loss of ions at metal surfaces: Band-structure effects. <i>Physical Review A</i> , 2003 , 67,	2.6	26
83	Electronic Stopping of Slow Protons in Oxides: Scaling Properties. <i>Physical Review Letters</i> , 2017 , 119, 163401	7.4	24

82	Vibrational Excitation of H Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 13617-13633	3.8	22
81	Femtosecond laser induced desorption of H ₂ , D ₂ , and HD from Ru(0001): Dynamical promotion and suppression studied with ab initio molecular dynamics with electronic friction. <i>Physical Review B</i> , 2017 , 95,	3.3	22
80	Influence of the van der Waals interaction in the dissociation dynamics of N ₂ on W(110) from first principles. <i>Journal of Chemical Physics</i> , 2015 , 142, 074704	3.9	22
79	Ab initio molecular dynamics study of the Eley-Rideal reaction of H + Cl-Au(111) → HCl + Au(111): Impact of energy dissipation to surface phonons and electron-hole pairs. <i>Journal of Chemical Physics</i> , 2018 , 148, 014702	3.9	22
78	Role of molecular electronic structure in inelastic electron tunneling spectroscopy: O ₂ on Ag(110). <i>Physical Review B</i> , 2010 , 82,	3.3	22
77	Electron-Mediated Phonon-Phonon Coupling Drives the Vibrational Relaxation of CO on Cu(100). <i>Physical Review Letters</i> , 2018 , 120, 156804	7.4	21
76	Dissociative dynamics of O ₂ on Ag(110). <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 9436-45	3.6	21
75	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 2287-2299	3.8	21
74	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 9779-9790	3.8	20
73	Non-reactive scattering of N ₂ from the W(110) surface studied with different exchange-correlation functionals. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 4357-64	3.6	20
72	Auger capture rates for a slow ion close to a metal surface. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1992 , 67, 157-159	1.2	20
71	Ultrafast Transient Dynamics of Adsorbates on Surfaces Deciphered: The Case of CO on Cu(100). <i>Physical Review Letters</i> , 2019 , 122, 016806	7.4	19
70	Diffusion of hydrogen in Pd assisted by inelastic ballistic hot electrons. <i>Physical Review Letters</i> , 2012 , 108, 115902	7.4	18
69	Auger deexcitation in a helium atom induced by a metal surface. <i>Physical Review A</i> , 1996 , 53, 4222-4227	2.6	18
68	Modeling surface motion effects in N ₂ dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model. <i>Journal of Chemical Physics</i> , 2016 , 144, 244708	3.9	18
67	Energy loss in gas-surface dynamics: Electron-hole pair and phonon excitation upon adsorbate relaxation. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2016 , 382, 26-31	1.2	16
66	Energy loss and surface temperature effects in ab initio molecular dynamics simulations: N adsorption on Ag(111) as a case study. <i>Physical Review B</i> , 2017 , 96,	3.3	16
65	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). <i>Physical Review B</i> , 2019 , 100,	3.3	16

64	Molecular dynamics simulation of O adsorption on Ag(110) from first principles electronic structure calculations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27366-27376	3.6	14
63	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2016 , 382, 114-118	1.2	14
62	Communication: Fingerprints of reaction mechanisms in product distributions: Eley-Rideal-type reactions between D and CD/Cu(111). <i>Journal of Chemical Physics</i> , 2018 , 149, 031101	3.9	14
61	Ready, Set and no Action: A Static Perspective on Potential Energy Surfaces commonly used in Gas-Surface Dynamics. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013 , 227,	3.1	14
60	The role of an electronic surface state in the stopping power of a swift charged particle in front of a metal. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 304209	1.8	14
59	Spin-dependent electron emission from metals in the neutralization of He ⁺ ions. <i>Physical Review A</i> , 2005 , 72,	2.6	14
58	CO Stretch Vibration Lives Long on Au(111). <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1043-1047	6.4	14
57	Stereodynamics of Diatom Formation through Eley-Rideal Abstraction. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 19849-19858	3.8	13
56	Dynamics of Nitrogen Scattering off N-Covered Ag(111). <i>Journal of Physical Chemistry C</i> , 2012 , 116, 21903-21913	3.8	13
55	Auger intra-atomic transitions in grazing atom-surface collisions. <i>Physical Review B</i> , 1994 , 49, 14589-14598	3.8	13
54	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. <i>Intermetallics</i> , 2019 , 106, 130-140	3.5	12
53	Dissociative adsorption of N ₂ on W(1 1 0): Theoretical study of the dependence on the incidence angle. <i>Surface Science</i> , 2007 , 601, 3726-3730	1.8	12
52	Spin-polarized electron excitation during the neutralization of He ⁺ ions in metals. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2004 , 137-140, 401-405	1.7	12
51	Effect of surface band structure in the energy loss of ions at surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2002 , 193, 585-589	1.2	11
50	Communication: Hot-atom abstraction dynamics of hydrogen from tungsten surfaces: The role of surface structure. <i>Journal of Chemical Physics</i> , 2017 , 147, 121103	3.9	10
49	Vibrational response and motion of carbon monoxide on Cu(100) driven by femtosecond laser pulses: Molecular dynamics with electronic friction. <i>Physical Review B</i> , 2019 , 100,	3.3	10
48	Electrons and Phonons Cooperate in the Laser-Induced Desorption of CO from Pd(111). <i>Physical Review Letters</i> , 2019 , 123, 246802	7.4	10
47	Time-dependent screening in a two-dimensional electron gas. <i>Surface Science</i> , 2004 , 559, 233-240	1.8	9

46	Time-dependent image potential at a metal surface. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003 , 129, 105-109	1.7	9
45	Ab Initio Molecular Dynamics Study of Alignment-Resolved O ₂ Scattering from Highly Oriented Pyrolytic Graphite. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 31094-31102	3.8	9
44	Role of valence states of adsorbates in inelastic electron tunneling spectroscopy: A study of nitric oxide on Cu(110) and Cu(001). <i>Physical Review B</i> , 2016 , 94,	3.3	8
43	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 20756-20762	3.8	8
42	Dynamic screening and electron dynamics in low-dimensional metal systems. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 258, 72-78	1.2	8
41	Role of the bound-state wave function in capture-loss rates: Slow proton in an electron gas. <i>Physical Review A</i> , 2003 , 68,	2.6	8
40	Photoinduced Desorption Dynamics of CO from Pd(111): A Neural Network Approach. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4648-4659	6.4	8
39	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15236-15243	3.8	7
38	The dynamics of adsorption and dissociation of N ₂ in a monolayer of iron on W(110). <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 19432-45	3.6	7
37	Minimum dipole moment required to bind an electron to a screened dipole field. <i>Physical Review B</i> , 2003 , 67,	3.3	7
36	Relaxation of excited electrons in a paramagnetic electron gas: The role of spins in screening and scattering. <i>Physical Review B</i> , 2001 , 64,	3.3	7
35	Spin effects in the screening and Auger neutralization of He ⁺ ions in a spin-polarized electron gas. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 230, 431-437	1.2	6
34	Band-structure-based collisional model for electronic excitations in ion-surface collisions. <i>Physical Review A</i> , 2005 , 72,	2.6	6
33	Dielectric response of covered metal surfaces: Oxidation of Al(111). <i>Physical Review B</i> , 2001 , 64,	3.3	6
32	Relaxation of excited electrons in an electron gas: A mean-field approach with charge and spin polarizations. <i>Physical Review B</i> , 2002 , 65,	3.3	6
31	Angular distributions and rovibrational excitation of N ₂ molecules recombined on N-covered Ag(111) by the Eley-Rideal mechanism. <i>Catalysis Today</i> , 2015 , 244, 115-121	5.3	5
30	Energy dissipation to tungsten surfaces upon hot-atom and Eley-Rideal recombination of H. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 21334-21344	3.6	5
29	Radiative neutralization of small clusters impinging on solid surfaces. <i>Zeitschrift Für Physik D-Atoms Molecules and Clusters</i> , 1997 , 41, 143-150		5

28	Spin dependence in the neutralization of He ⁺ ions in metals: An analysis of different contributions. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 232, 8-15	1.2	5
27	Electron emission in the Auger neutralization of a spin-polarized He ⁺ ion embedded in a free electron gas. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 232, 73-78	1.2	5
26	Energy Dissipation Channels in Reactive and Non-reactive Scattering at Surfaces. <i>Springer Series in Surface Sciences</i> , 2013 , 371-388	0.4	5
25	High-Dimensional Atomistic Neural Network Potential to Study the Alignment-Resolved O Scattering From Highly Oriented Pyrolytic Graphite. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 2588-2600 ^{2.8}		5
24	Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations. <i>Journal of Applied Physics</i> , 2020 , 127, 145102	2.5	4
23	Two dimensional behaviour of friction at a metal surface with a surface state. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 256, 383-386	1.2	4
22	3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces. <i>Physical Review A</i> , 2007 , 76,	2.6	4
21	The relaxation rate in hot-electron dynamics: beyond the first-order Born approximation in kinetic theory. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, 7859-7865	1.8	4
20	Energy Loss in the Interaction of Atomic Particles with Solid Surfaces. <i>Advances in Quantum Chemistry</i> , 2004 , 223-245	1.4	4
19	Nonlinear effects in the energy loss of a slow dipole in a free-electron gas. <i>Physical Review A</i> , 2002 , 66,	2.6	4
18	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)]. <i>Physical Review Letters</i> , 2012 , 108,	7.4	3
17	Interaction of slow multicharged ions with surfaces. <i>Radiation Physics and Chemistry</i> , 2007 , 76, 412-417	2.5	3
16	Spin polarization effects in the interaction of light atoms with a free electron gas. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003 , 129, 207-211	1.7	3
15	Ion induced electronic excitations in a spin-polarized electron gas. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003 , 203, 83-88	1.2	2
14	Relaxation rate of excited electrons in an electron gas. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003 , 129, 117-126	1.7	2
13	Spin dependent screening and Auger neutralization of singly-charged noble gas ions in metals. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 256, 24-29	1.2	1
12	Spin-dependent electron excitation and emission in the neutralization of He ⁺ ions at paramagnetic surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 256, 423-428	1.2	1
11	Vicinage effects in the energy loss of slow LiH molecules in metals. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 232, 178-183	1.2	1

10	Auger deexcitation rates in grazing atom-surface collisions. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1995 , 98, 424-428	1.2	1
9	Insights into the Coadsorption and Reactivity of O and CO on Ru(0001) and Their Coverage Dependence. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 12614-12627	3.8	1
8	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. <i>Applied Surface Science</i> , 2021 , 559, 149835	6.7	1
7	Absence of isotope effects in the photo-induced desorption of CO from saturated Pd(111) at high laser fluence. <i>Chemical Physics</i> , 2022 , 558, 111518	2.3	1
6	Photon emission from Ag _n ⁺ clusters: Role of the ionization potential. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1997 , 125, 7-12	1.2	
5	Influence of plasmon-assisted charge exchange processes on ion-induced electron emission from metals. <i>Vacuum</i> , 2006 , 80, 554-560	3.7	
4	Surface photoelectric effect induced by small clusters impinging on solid surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2000 , 164-165, 662-670	1.2	
3	Nonadiabatic Effects in Gas-Surface Dynamics. <i>Springer Handbooks</i> , 2020 , 929-965	1.3	
2	Spin Polarization of Electrons Emitted in the Neutralization of He ⁺ Ions in Solids 2007 , 153-183		
1	O ₂ on Ag(110): A puzzle for exchange-correlation functionals. <i>Chemical Physics</i> , 2021 , 554, 111424	2.3	