Maite Alducin

List of Publications by Year
in descending order

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118 papers	2,759 citations	172207 29 h-index	223531 46 g-index
124 all docs	124 docs citations	124 times ranked	1000 citing authors

#	Article	IF	Citations
1	Role of Electron-Hole Pair Excitations in the Dissociative Adsorption of Diatomic Molecules on Metal Surfaces. Physical Review Letters, 2008, 100, 116102.	2.9	231
2	Electronic Friction Dominates Hydrogen Hot-Atom Relaxation on Pd(100). Physical Review Letters, 2014, 112, 103203.	2.9	112
3	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.	2.9	79
4	Non-adiabatic effects in elementary reaction processes at metal surfaces. Progress in Surface Science, 2017, 92, 317-340.	3.8	79
5	Ab initiomolecular dynamics with simultaneous electron and phonon excitations: Application to the relaxation of hot atoms and molecules on metal surfaces. Physical Review B, 2015, 92, .	1.1	76
6	WhyN2Molecules with Thermal Energy Abundantly Dissociate on W(100) and Not on W(110). Physical Review Letters, 2006, 97, 056102.	2.9	75
7	Electronâ€“Hole Pair Effects in Polyatomic Dissociative Chemisorption: Water on Ni(111). Journal of Physical Chemistry Letters, 2016, 7, 327-331.	2.1	68
8	Surface electron density models for accurateab initiomolecular dynamics with electronic friction. Physical Review B, 2016, 93, .	1.1	54
9	Local theory of Auger neutralization for slow and compact ions interacting with metal surfaces. Physical Review A, 1994, 49, 4716-4725.	1.0	52
10	Electronic Stopping of Slow Protons in Transition and Rare Earth Metals: Breakdown of the Free Electron Gas Concept. Physical Review Letters, 2017, 118, 103401.	2.9	52
11	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). Journal of Chemical Physics, 2016, 145, 044704.	1.2	51
12	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. Journal of Physical Chemistry C, 2016, 120, 17357-17364.	1.5	51
13	The role of exchange-correlation functionals in the potential energy surface and dynamics of N2 dissociation on W surfaces. Journal of Chemical Physics, 2008, 128, 154704.	1.2	48
14	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.	1.2	48
15	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.	2.1	44
16	Low sticking probability in the nonactivated dissociation of N2 molecules on W(110). Journal of Chemical Physics, 2006, 125, 144705.	1.2	42
17	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). Physical Review B, 2016, 93, .	1.1	42
18	Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111). Journal of Chemical Physics, 2014, 141, 054705.	1.2	41

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19	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.	1.2	40
20	Vibrational lifetimes of hydrogen on lead films: An ab initio molecular dynamics with electronic friction (AIMDEF) study. Journal of Chemical Physics, 2014, 141, 234702.	1.2	40
21	Energy Dissipation to Tungsten Surfaces upon Eleyâ€“Rideal Recombination of N₂ and H₂. Journal of Physical Chemistry C, 2015, 119, 15434-15442.	1.5	40
22	Dissociative dynamics of spin-triplet and spin-singlet O2 on Ag(100). Journal of Chemical Physics, 2008, 129, 224702.	1.2	39
23	Mixed-Valency Signature in Vibrational Inelastic Electron Tunneling Spectroscopy. Physical Review Letters, 2010, 104, 136101.	2.9	39
24	Dissociative and non-dissociative adsorption dynamics of N2 on Fe(110). Physical Chemistry Chemical Physics, 2012, 14, 7471.	1.3	37
25	Electronic Stopping of Slow Protons in Oxides: Scaling Properties. Physical Review Letters, 2017, 119, 163401.	2.9	34
26	Surface Strain Improves Molecular Adsorption but Hampers Dissociation for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Fe</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi mat	2.9	33
27	Efficient N₂ Formation on Ag(111) by Eleyâ€“Rideal Recombination of Hyperthermal Atoms. Journal of Physical Chemistry Letters, 2013, 4, 3704-3709.	2.1	32
28	Effects of electronic relaxation processes on vibrational linewidths of adsorbates on surfaces: The case of CO/Cu(100). Physical Review B, 2016, 94, .	1.1	31
29	Dissipative effects in the dynamics of N₂on tungsten surfaces. Journal of Physics Condensed Matter, 2009, 21, 264007.	0.7	30
30	Hydrogen abstraction from metal surfaces: when electronâ€“hole pair excitations strongly affect hot-atom recombination. Physical Chemistry Chemical Physics, 2016, 18, 31378-31383.	1.3	30
31	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 2287-2299.	1.5	30
32	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. Intermetallics, 2019, 106, 130-140.	1.8	29
33	Ultrafast Transient Dynamics of Adsorbates on Surfaces Deciphered: The Case of CO on Cu(100). Physical Review Letters, 2019, 122, 016806.	2.9	29
34	JuaristietÂal.Reply:. Physical Review Letters, 2009, 102, .	2.9	28
35	Energy dissipation channels in the adsorption of N on Ag(111). Computational and Theoretical Chemistry, 2012, 990, 126-131.	1.1	28
36	Energy loss of ions at metal surfaces: Band-structure effects. Physical Review A, 2003, 67, .	1.0	27

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37	Spin-dependent screening and Auger neutralization ofHe+ions in metals. Physical Review A, 2004, 70, .	1.0	27
38	Role of Physisorption States in Molecular Scattering: A Semilocal Density-Functional Theory Study on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 682 Td (stretchy="false">)</mml:mo></mml:mrow></mml:math>	2.9	27
39	Vibrational Excitation of H₂ 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.	1.5	26
40	Femtosecond laser induced desorption of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>,</mml:mo><mml:msub><mml:mi mathvariant="normal">D</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> , and HD from Ru(0001): Dynamical promotion and suppression studied with ab initio molecular dynamics with electronic friction. Physical Review B, 2017, 95, .	1.1	26
41	Electron-Mediated Phonon-Phonon Coupling Drives the Vibrational Relaxation of CO on Cu(100). Physical Review Letters, 2018, 120, 156804.	2.9	26
42	Ab initio molecular dynamics study of the Eley-Rideal reaction of H + Clâ€“Au(111) â†’ HCl + Au(111): Impact of energy dissipation to surface phonons and electron-hole pairs. Journal of Chemical Physics, 2018, 148, 014702.	1.2	25
43	Role of molecular electronic structure in inelastic electron tunneling spectroscopy:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Ag(110). Physical Review B, 2010, 82, .	1.1	24
44	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.	1.2	23
45	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). Physical Review B, 2019, 100, .	1.1	23
46	Dissociative dynamics of O₂ on Ag(110). Physical Chemistry Chemical Physics, 2015, 17, 9436-9445.	1.3	22
47	CO Stretch Vibration Lives Long on Au(111). Journal of Physical Chemistry Letters, 2019, 10, 1043-1047.	2.1	21
48	Auger capture rates for a slow ion close to a metal surface. Nuclear Instruments & Methods in Physics Research B, 1992, 67, 157-159.	0.6	20
49	Non-reactive scattering of N2 from the W(110) surface studied with different exchangeâ€“correlation functionals. Physical Chemistry Chemical Physics, 2011, 13, 4357.	1.3	20
50	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 9779-9790.	1.5	20
51	Diffusion of Hydrogen in Pd Assisted by Inelastic Ballistic Hot Electrons. Physical Review Letters, 2012, 108, 115902.	2.9	19
52	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.	1.2	19
53	Energy loss in gas-surface dynamics: Electronâ€“hole pair and phonon excitation upon adsorbate relaxation. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 26-31.	0.6	19
54	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, .	1.1	19

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55	Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations. Journal of Applied Physics, 2020, 127, .	1.1	19
56	Auger deexcitation in a helium atom induced by a metal surface. Physical Review A, 1996, 53, 4222-4227.	1.0	18
57	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 114-118.	0.6	18
58	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	3.1	17
59	Communication: Fingerprints of reaction mechanisms in product distributions: Eley-Rideal-type reactions between D and CD3/Cu(111). Journal of Chemical Physics, 2018, 149, 031101.	1.2	16
60	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, .	1.1	16
61	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.	0.7	15
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, .	1.4	15
63	Stereodynamics of Diatom Formation through Eleyâ€“Rideal Abstraction. Journal of Physical Chemistry C, 2017, 121, 19849-19858.	1.5	15
64	Ab Initio Molecular Dynamics Study of Alignment-Resolved O₂ Scattering from Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry C, 2019, 123, 31094-31102.	1.5	15
65	Electrons and Phonons Cooperate in the Laser-Induced Desorption of CO from Pd(111). Physical Review Letters, 2019, 123, 246802.	2.9	15
66	Photoinduced Desorption Dynamics of CO from Pd(111): A Neural Network Approach. Journal of Chemical Theory and Computation, 2021, 17, 4648-4659.	2.3	15
67	Spin-dependent electron emission from metals in the neutralization ofHe+ions. Physical Review A, 2005, 72, .	1.0	14
68	Dynamics of Nitrogen Scattering off N-Covered Ag(111). Journal of Physical Chemistry C, 2012, 116, 21903-21912.	1.5	14
69	Molecular dynamics simulation of O₂ adsorption on Ag(110) from first principles electronic structure calculations. Physical Chemistry Chemical Physics, 2016, 18, 27366-27376.	1.3	14
70	Auger intra-atomic transitions in grazing atom-surface collisions. Physical Review B, 1994, 49, 14589-14598.	1.1	13
71	Dissociative adsorption of N2 on W(110): Theoretical study of the dependence on the incidence angle. Surface Science, 2007, 601, 3726-3730.	0.8	13
72	Spin-polarized electron excitation during the neutralization of He+ ions in metals. Journal of Electron Spectroscopy and Related Phenomena, 2004, 137-140, 401-405.	0.8	12

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73	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, .	1.1	12
74	Communication: Hot-atom abstraction dynamics of hydrogen from tungsten surfaces: The role of surface structure. Journal of Chemical Physics, 2017, 147, 121103.	1.2	12
75	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. Journal of Physical Chemistry C, 2017, 121, 20756-20762.	1.5	12
76	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. Journal of Physical Chemistry C, 2019, 123, 15236-15243.	1.5	12
77	Effect of surface band structure in the energy loss of ions at surfaces. Nuclear Instruments & Methods in Physics Research B, 2002, 193, 585-589.	0.6	11
78	Time-dependent image potential at a metal surface. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 105-109.	0.8	9
79	Role of the bound-state wave function in capture-loss rates: Slow proton in an electron gas. Physical Review A, 2003, 68, .	1.0	9
80	Time-dependent screening in a two-dimensional electron gas. Surface Science, 2004, 559, 233-240.	0.8	9
81	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.	1.5	9
82	Dielectric response of covered metal surfaces: Oxidation of Al(111). Physical Review B, 2001, 64, .	1.1	8
83	Relaxation of excited electrons in a paramagnetic electron gas: The role of spins in screening and scattering. Physical Review B, 2001, 64, .	1.1	8
84	Dynamic screening and electron dynamics in low-dimensional metal systems. Nuclear Instruments & Methods in Physics Research B, 2007, 258, 72-78.	0.6	8
85	High-Dimensional Atomistic Neural Network Potential to Study the Alignment-Resolved O2 Scattering from Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry A, 2021, 125, 2588-2600.	1.1	8
86	Minimum dipole moment required to bind an electron to a screened dipole field. Physical Review B, 2003, 67, .	1.1	7
87	The dynamics of adsorption and dissociation of N2 in a monolayer of iron on W(110). Physical Chemistry Chemical Physics, 2015, 17, 19432-19445.	1.3	7
88	Energy dissipation to tungsten surfaces upon hot-atom and Eleyâ€“Rideal recombination of H₂. Physical Chemistry Chemical Physics, 2018, 20, 21334-21344.	1.3	7
89	Relaxation of excited electrons in an electron gas: A mean-field approach with charge and spin polarizations. Physical Review B, 2002, 65, .	1.1	6
90	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.	0.6	6

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91	Band-structure-based collisional model for electronic excitations in ion-surface collisions. Physical Review A, 2005, 72, .	1.0	6
92	Radiative neutralization of small clusters impinging on solid surfaces. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 41, 143-150.	1.0	5
93	Nonlinear effects in the energy loss of a slow dipole in a free-electron gas. Physical Review A, 2002, 66, .	1.0	5
94	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.	0.6	5
95	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.	0.6	5
96	Angular distributions and rovibrational excitation of N2 molecules recombined on N-covered Ag(111) by the Eleyâ€“Rideal mechanism. Catalysis Today, 2015, 244, 115-121.	2.2	5
97	Energy Dissipation Channels in Reactive and Non-reactive Scattering at Surfaces. Springer Series in Surface Sciences, 2013, , 371-388.	0.3	5
98	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.	0.7	4
99	Energy Loss in the Interaction of Atomic Particles with Solid Surfaces. Advances in Quantum Chemistry, 2004, , 223-245.	0.4	4
100	3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces. Physical Review A, 2007, 76, .	1.0	4
101	Two dimensional behaviour of friction at a metal surface with a surface state. Nuclear Instruments & Methods in Physics Research B, 2007, 256, 383-386.	0.6	4
102	Interaction of slow multicharged ions with surfaces. Radiation Physics and Chemistry, 2007, 76, 412-417.	1.4	4
103	Spinâ€“polarization effects in the interaction of light atoms with a free electron gas. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 207-211.	0.8	3
104	Publisherâ€™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, .	2.9	3
105	Adsorption and dissociation of diatomic molecules on monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>H</mml:mi></mml:mrow><mml:mn> Physical Review B, 2022, 105, .	1.1	3
106	Absence of isotope effects in the photo-induced desorption of CO from saturated Pd(111) at high laser fluence. Chemical Physics, 2022, 558, 111518.	0.9	3
107	Ion induced electronic excitations in a spin-polarized electron gas. Nuclear Instruments & Methods in Physics Research B, 2003, 203, 83-88.	0.6	2
108	Relaxation rate of excited electrons in an electron gas. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 117-126.	0.8	2

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109	Auger deexcitation rates in grazing atom-surface collisions. Nuclear Instruments & Methods in Physics Research B, 1995, 98, 424-428.	0.6	1
110	Vicinage effects in the energy loss of slow LiH molecules in metals. Nuclear Instruments & Methods in Physics Research B, 2005, 232, 178-183.	0.6	1
111	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.	0.6	1
112	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.	0.6	1
113	Nonadiabatic Effects in Gas-Surface Dynamics. Springer Handbooks, 2020, , 929-965.	0.3	1
114	Photon emission from Agn+ clusters: Role of the ionization potential. Nuclear Instruments & Methods in Physics Research B, 1997, 125, 7-12.	0.6	0
115	Surface photoelectric effect induced by small clusters impinging on solid surfaces. Nuclear Instruments & Methods in Physics Research B, 2000, 164-165, 662-670.	0.6	0
116	Influence of plasmon-assisted charge exchange processes on ion-induced electron emission from metals. Vacuum, 2006, 80, 554-560.	1.6	0
117	Preface: Proceedings of the 21st International Workshop on Inelastic Ion-Surface Collisions (IISC-21). Nuclear Instruments & Methods in Physics Research B, 2016, 382, 1.	0.6	0
118	O2 on Ag(110): A puzzle for exchange-correlation functionals. Chemical Physics, 2021, 554, 111424.	0.9	0