

Joseba Iñai Juaristi

List of Publications by Year in descending order

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137
docs citations

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1156
citing authors

#	ARTICLE	IF	CITATIONS
1	Role of Electron-Hole Pair Excitations in the Dissociative Adsorption of Diatomic Molecules on Metal Surfaces. <i>Physical Review Letters</i> , 2008, 100, 116102.	2.9	231
2	Electronic Stopping Power in LiF from First Principles. <i>Physical Review Letters</i> , 2007, 99, 235501.	2.9	157
3	Electronic Stopping Power in Gold: The Role of d Electrons and the H -He Anomaly. <i>Physical Review Letters</i> , 2012, 108, 225504.	2.9	125
4	Electronic Friction Dominates Hydrogen Hot-Atom Relaxation on Pd(100). <i>Physical Review Letters</i> , 2014, 112, 103203.	2.9	112
5	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.	2.9	79
6	Non-adiabatic effects in elementary reaction processes at metal surfaces. <i>Progress in Surface Science</i> , 2017, 92, 317-340.	3.8	79
7	Charge State Dependence of the Energy Loss of Slow Ions in Metals. <i>Physical Review Letters</i> , 1999, 82, 1048-1051.	2.9	77
8	<i>Ab initio</i> 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, .	1.1	76
9	Electronic Friction-Based Vibrational Lifetimes of Molecular Adsorbates: Beyond the Independent-Atom Approximation. <i>Physical Review Letters</i> , 2015, 115, 046102.	2.9	65
10	Unexpected Behavior of the Stopping of Slow Ions in Ionic Crystals. <i>Physical Review Letters</i> , 2000, 84, 2124-2127.	2.9	56
11	Energy loss of slow ions in a nonuniform electron gas. <i>Physical Review B</i> , 2003, 67, .	1.1	55
12	Surface electron density models for accurate <i>ab initio</i> molecular dynamics with electronic friction. <i>Physical Review B</i> , 2016, 93, .	1.1	54
13	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.	2.9	52
14	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). <i>Journal of Chemical Physics</i> , 2016, 145, 044704.	1.2	51
15	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.	1.5	51
16	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.	1.2	48
17	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). <i>Physical Review B</i> , 2016, 93, .	1.1	42
18	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.	1.2	40

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19	Vibrational lifetimes of hydrogen on lead films: An <i>ab initio</i> molecular dynamics with electronic friction (AIMDEF) study. <i>Journal of Chemical Physics</i> , 2014, 141, 234702.	1.2	40
20	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.	1.5	40
21	Energy loss of MeV protons specularly reflected from metal surfaces. <i>Physical Review B</i> , 1996, 53, 13839-13850.	1.1	37
22	Dissociative and non-dissociative adsorption dynamics of N_2 on Fe(110). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7471.	1.3	37
23	Channeling effects observed in energy-loss spectra of nitrogen ions scattered off a Pt(110) surface. <i>Physical Review A</i> , 2001, 64, .	1.0	35
24	Electronic Stopping of Slow Protons in Oxides: Scaling Properties. <i>Physical Review Letters</i> , 2017, 119, 163401.	2.9	34
25	Surface Strain Improves Molecular Adsorption but Hampers Dissociation for N_2 on $Fe(110)$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15434-15442.	1.5	34
26	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.	2.1	32
27	Crystal Effects in the Neutralization of He^+ Ions in the Low Energy Ion Scattering Regime. <i>Physical Review Letters</i> , 2008, 100, 213201.	2.9	31
28	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, .	1.1	31
29	Dissipative effects in the dynamics of N_2 on tungsten surfaces. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 264007.	0.7	30
30	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.	1.3	30
31	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.	1.5	30
32	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. <i>Intermetallics</i> , 2019, 106, 130-140.	1.8	29
33	Ultrafast Transient Dynamics of Adsorbates on Surfaces Deciphered: The Case of CO on Cu(100). <i>Physical Review Letters</i> , 2019, 122, 016806.	2.9	29
34	Nonlinear screening effects in the interaction of slow multicharged ions with metal surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1995, 100, 279-283.	0.6	28
35	Juaristiet Al.Reply.. <i>Physical Review Letters</i> , 2009, 102, .	2.9	28
36	Energy dissipation channels in the adsorption of N on Ag(111). <i>Computational and Theoretical Chemistry</i> , 2012, 990, 126-131.	1.1	28

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37	Femtosecond-laser induced dynamics of CO on Ru(0001): Deep insights from a hot-electron friction model including surface motion. <i>Physical Review B</i> , 2016, 94, .	1.1	28
38	Energy loss of ions at metal surfaces: Band-structure effects. <i>Physical Review A</i> , 2003, 67, .	1.0	27
39	Spin-dependent screening and Auger neutralization of He ⁺ ions in metals. <i>Physical Review A</i> , 2004, 70, .	1.0	27
40	Role of Physisorption States in Molecular Scattering: A Semilocal Density-Functional Theory Study on O scattering from Cu(111). <i>Physical Review B</i> , 2017, 95, .	2.9	27
41	Vibrational Excitation of H ₂ 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.	1.5	26
42	Femtosecond laser induced desorption of H ₂ from Cu(111): Dynamical promotion and suppression studied with <i>ab initio</i> molecular dynamics with electronic friction. <i>Physical Review B</i> , 2017, 95, .	1.1	26
43	Electron-Mediated Phonon-Phonon Coupling Drives the Vibrational Relaxation of CO on Cu(100). <i>Physical Review Letters</i> , 2018, 120, 156804.	2.9	26
44	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.	1.2	23
45	Electronic stopping power of Al ₂ O ₃ and SiO ₂ for H, He, and N. <i>Physical Review A</i> , 2001, 64, .	1.0	22
46	Dissociative dynamics of O ₂ on Ag(110). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9436-9445.	1.3	22
47	CO Stretch Vibration Lives Long on Au(111). <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1043-1047.	2.1	21
48	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.	1.3	20
49	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9779-9790.	1.5	20
50	Charge state dependence of the energy loss of slow nitrogen ions reflected from an aluminum surface under grazing incidence. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1999, 157, 87-91.	0.6	19
51	Diffusion of Hydrogen in Pd Assisted by Inelastic Ballistic Hot Electrons. <i>Physical Review Letters</i> , 2012, 108, 115902.	2.9	19
52	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.	0.6	19
53	Energy loss and surface temperature effects in <i>ab initio</i> molecular dynamics simulations: N adsorption on Ag(111) as a case study. <i>Physical Review B</i> , 2017, 96, .	1.1	19
54	Structure and properties of CoCrFeNiX multi-principal element alloys from <i>ab initio</i> calculations. <i>Journal of Applied Physics</i> , 2020, 127, .	1.1	19

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55	Contribution of the excitation of conduction band electrons to the kinetic electron emission induced by slow ions in metals. <i>Physical Review B</i> , 1998, 58, 15838-15846.	1.1	18
56	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2016, 382, 114-118.	0.6	18
57	Strong Anisotropic Interaction Controls Unusual Sticking and Scattering of CO at Ru(0001). <i>Physical Review Letters</i> , 2017, 119, 146101.	2.9	17
58	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. <i>Applied Surface Science</i> , 2021, 559, 149835.	3.1	17
59	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, .	1.1	16
60	Interaction of multiply charged ions with metals. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1996, 115, 173-176.	0.6	15
61	Short-range correlation in an electron gas: A scattering approach. <i>Physical Review B</i> , 2003, 67, .	1.1	15
62	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.	0.7	15
63	Stereodynamics of Diatom Formation through Eley-Rideal Abstraction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19849-19858.	1.5	15
64	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.	1.5	15
65	Electrons and Phonons Cooperate in the Laser-Induced Desorption of CO from Pd(111). <i>Physical Review Letters</i> , 2019, 123, 246802.	2.9	15
66	Photoinduced Desorption Dynamics of CO from Pd(111): A Neural Network Approach. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4648-4659.	2.3	15
67	Spin-dependent electron emission from metals in the neutralization of He ⁺ ions. <i>Physical Review A</i> , 2005, 72, .	1.0	14
68	Dynamics of Nitrogen Scattering off N-Covered Ag(111). <i>Journal of Physical Chemistry C</i> , 2012, 116, 21903-21912.	1.5	14
69	Molecular dynamics simulation of O_2 adsorption on Ag(110) from first principles electronic structure calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27366-27376.	1.3	14
70	Energy loss of fast protons specularly reflected from metal surfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1999, 157, 104-109.	0.6	12
71	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.	0.8	12
72	LEIS: A reliable tool for surface composition analysis?. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009, 267, 624-627.	0.6	12

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73	Communication: Hot-atom abstraction dynamics of hydrogen from tungsten surfaces: The role of surface structure. <i>Journal of Chemical Physics</i> , 2017, 147, 121103.	1.2	12
74	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.	1.5	12
75	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15236-15243.	1.5	12
76	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.	0.6	11
77	Relaxation rate of excited electrons in metals: A nonperturbative calculation based on kinetic theory. <i>Physical Review B</i> , 2000, 63, .	1.1	10
78	Dynamics of N ₂ sticking on W(100): the decisive role of van der Waals interactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19326-19331.	1.3	10
79	Energy loss in grazing proton-surface collisions. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1994, 90, 252-256.	0.6	9
80	Time-dependent image potential at a metal surface. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003, 129, 105-109.	0.8	9
81	Trajectory straggling and nonlinear effects in the energy loss of surface-channeled ions. <i>Physical Review B</i> , 2003, 67, .	1.1	9
82	Spin-resolved pair-distribution functions in an electron gas: A scattering approach based on consistent potentials. <i>Physical Review B</i> , 2004, 69, .	1.1	9
83	Time-dependent screening in a two-dimensional electron gas. <i>Surface Science</i> , 2004, 559, 233-240.	0.8	9
84	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.	1.5	9
85	Projectile charge dependence of kinetic electron emission from clean gold. <i>Physica Scripta</i> , 1997, T73, 322-323.	1.2	8
86	Nonlinear effects in the kinetic electron emission induced by slow ions in metals. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1998, 135, 487-491.	0.6	8
87	Relaxation of excited electrons in a paramagnetic electron gas: The role of spins in screening and scattering. <i>Physical Review B</i> , 2001, 64, .	1.1	8
88	Charge-state dependence of kinetic electron emission induced by slow ions in metals. <i>Physical Review A</i> , 2003, 68, .	1.0	8
89	Quantum-size effects in the energy loss of charged particles interacting with a confined two-dimensional electron gas. <i>Physical Review A</i> , 2006, 73, .	1.0	8
90	Dynamic screening and electron dynamics in low-dimensional metal systems. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007, 258, 72-78.	0.6	8

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91	High-Dimensional Atomistic Neural Network Potential to Study the Alignment-Resolved O ₂ Scattering from Highly Oriented Pyrolytic Graphite. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2588-2600.	1.1	8
92	Energy-loss contribution to grazing scattering of fast He atoms from a silver surface. <i>Physical Review A</i> , 2014, 89, .	1.0	7
93	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, 19432-19445.	1.3	7
94	Energy dissipation to tungsten surfaces upon hot-atom and Eley-Rideal recombination of H ₂ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21334-21344.	1.3	7
95	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.	0.6	6
96	Band-structure-based collisional model for electronic excitations in ion-surface collisions. <i>Physical Review A</i> , 2005, 72, .	1.0	6
97	Transport cross sections based on a screened interaction potential: Comparison of classical and quantum-mechanical results. <i>Physical Review A</i> , 2005, 71, .	1.0	6
98	Electronic friction coefficients from the atom-in-jellium model for $Z \ll 1$. <i>Physical Review B</i> , 2020, 102, .		
99	Consistent model for the screening of slow muons in metals. <i>Physical Review B</i> , 1999, 60, R12546-R12548.	1.1	5
100	Nonlinear effects in the energy loss of a slow dipole in a free-electron gas. <i>Physical Review A</i> , 2002, 66, .	1.0	5
101	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.	0.6	5
102	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.	2.2	5
103	Energy Dissipation Effects on the Adsorption Dynamics of N ₂ on W(100). <i>Journal of Physical Chemistry C</i> , 2019, 123, 2900-2910.	1.5	5
104	Energy Dissipation Channels in Reactive and Non-reactive Scattering at Surfaces. <i>Springer Series in Surface Sciences</i> , 2013, , 371-388.	0.3	5
105	Atomic number dependence of the forward/backward kinetic electron emission induced by slow ions in carbon foils. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1999, 157, 254-258.	0.6	4
106	Molecular projectile effects for kinetic electron emission from carbon- and metal-surfaces bombarded by slow hydrogen ions. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003, 203, 1-7.	0.6	4
107	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.	0.7	4
108	Energy Loss in the Interaction of Atomic Particles with Solid Surfaces. <i>Advances in Quantum Chemistry</i> , 2004, , 223-245.	0.4	4

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109	Energy loss of ions interacting with metal surfaces. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 148-157.	0.6	4
110	3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces. Physical Review A, 2007, 76, .	1.0	4
111	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
112	Interaction of slow multicharged ions with surfaces. Radiation Physics and Chemistry, 2007, 76, 412-417.	1.4	4
113	Energy-loss straggling of swift heavy ions in an electron gas. Physical Review A, 2008, 78, .	1.0	4
114	Heating electrons with ion irradiation: A first-principles approach. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 590-593.	0.6	4
115	Transient metal-like electrical conductivity in swift heavy ion irradiated insulators. Nuclear Instruments & Methods in Physics Research B, 2013, 317, 72-76.	0.6	4
116	Coulomb explosion of H ₂ ⁺ in surface scattering. Nuclear Instruments & Methods in Physics Research B, 1998, 142, 473-485.	0.6	3
117	Spin 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
118	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, .	2.9	3
119	Adsorption and dissociation of diatomic molecules on monolayer H_2 . Physical Review B, 2022, 105, .	0.6	3
120	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
121	Ion induced electronic excitations in a spin-polarized electron gas. Nuclear Instruments & Methods in Physics Research B, 2003, 203, 83-88.	0.6	2
122	Relaxation rate of excited electrons in an electron gas. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 117-126.	0.8	2
123	Charge state dependent kinetic electron emission induced by slow Nq ⁺ ions in a spin-polarized electron gas. Nuclear Instruments & Methods in Physics Research B, 2005, 232, 67-72.	0.6	2
124	On the metallization of the LiF monolayer. Solid State Communications, 1994, 91, 957-960.	0.9	1
125	Charge transfer rates for excited states of protons at surfaces. Radiation Effects and Defects in Solids, 1994, null, 167-173.	0.4	1
126	Auger deexcitation rates in grazing atom-surface collisions. Nuclear Instruments & Methods in Physics Research B, 1995, 98, 424-428.	0.6	1

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127	Z1 oscillations in the spin polarization of electrons excited by slow ions in a spin-polarized electron gas. Nuclear Instruments & Methods in Physics Research B, 2007, 258, 79-82.	0.6	1
128	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
129	Trajectory-dependent energy loss for swift He atoms axially scattered off a silver surface. Nuclear Instruments & Methods in Physics Research B, 2014, 340, 15-20.	0.6	1
130	Electron-Hole Pairs in Surface Dynamics. , 2018, , 356-365.		1
131	Nonadiabatic Effects in Gas-Surface Dynamics. Springer Handbooks, 2020, , 929-965.	0.3	1
132	Energy-loss contribution for fast He atoms axially scattered off a silver surface. Journal of Physics: Conference Series, 2015, 635, 032013.	0.3	0
133	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
134	O2 on Ag(110): A puzzle for exchange-correlation functionals. Chemical Physics, 2021, 554, 111424.	0.9	0