Joseba IÃ±ai Juaristi

List of Publications by Year
in descending order

134	3,037	172386	206029
papers	citations	29 h-index	48 g-index

137	137	137	1156
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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	1.1	3
	Physical Review B, 2022, 105, .		
2	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
3	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
4	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
5	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
6	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	3.1	17
7	O2 on Ag(110): A puzzle for exchange-correlation functionals. Chemical Physics, 2021, 554, 111424.	0.9	0
8	Electronic friction coefficients from the atom-in-jellium model for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Z</mml:mi><mml:mo>=</mml:mo><mml:mn	1.1	1
	Physical Review B, 2020, 102, .		
9	Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations. Journal of Applied Physics, 2020, 127, .	1.1	19
10	Nonadiabatic Effects in Gas-Surface Dynamics. Springer Handbooks, 2020, , 929-965.	0.3	1
11	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. Intermetallics, 2019, 106, 130-140.	1.8	29
12	Energy Dissipation Effects on the Adsorption Dynamics of N2 on W(100). Journal of Physical Chemistry C, 2019, 123, 2900-2910.	1.5	5
13	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. Journal of Physical Chemistry C, 2019, 123, 15236-15243.	1.5	12
14	CO Stretch Vibration Lives Long on Au(111). Journal of Physical Chemistry Letters, 2019, 10, 1043-1047.	2.1	21
15	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
16	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
17	Electrons and Phonons Cooperate in the Laser-Induced Desorption of CO from Pd(111). Physical Review Letters, 2019, 123, 246802.	2.9	15
18	Ultrafast Transient Dynamics of Adsorbates on Surfaces Deciphered: The Case of CO on Cu(100). Physical Review Letters, 2019, 122, 016806.	2.9	29

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19	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
20	Electron-Mediated Phonon-Phonon Coupling Drives the Vibrational Relaxation of CO on Cu(100). Physical Review Letters, 2018, 120, 156804.	2.9	26
21	Electronâ€“Hole Pairs in Surface Dynamics. , 2018, , 356-365.		1
22	Dynamics of N2 sticking on W(100): the decisive role of van der Waals interactions. Physical Chemistry Chemical Physics, 2018, 20, 19326-19331.	1.3	10
23	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
24	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
25	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
26	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
27	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
28	Strong Anisotropic Interaction Controls Unusual Sticking and Scattering of CO at Ru(0001). Physical Review Letters, 2017, 119, 146101.	2.9	17
29	Non-adiabatic effects in elementary reaction processes at metal surfaces. Progress in Surface Science, 2017, 92, 317-340.	3.8	79
30	Stereodynamics of Diatom Formation through Eleyâ€“Rideal Abstraction. Journal of Physical Chemistry C, 2017, 121, 19849-19858.	1.5	15
31	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
32	Electronic Stopping of Slow Protons in Oxides: Scaling Properties. Physical Review Letters, 2017, 119, 163401.	2.9	34
33	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
34	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). Journal of Chemical Physics, 2016, 145, 044704.	1.2	51
35	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
36	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

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37	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
38	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
39	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). Physical Review B, 2016, 93, .	1.1	42
40	Surface electron density models for accurateab initiomolecular dynamics with electronic friction. Physical Review B, 2016, 93, .	1.1	54
41	Femtosecond-laser induced dynamics of CO on Ru(0001): Deep insights from a hot-electron friction model including surface motion. Physical Review B, 2016, 94, .	1.1	28
42	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
43	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
44	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 114-118.	0.6	18
45	Electronic Friction-Based Vibrational Lifetimes of Molecular Adsorbates: Beyond the Independent-Atom Approximation. Physical Review Letters, 2015, 115, 046102.	2.9	65
46	Energy-loss contribution for fast He atoms axially scattered off a silver surface. Journal of Physics: Conference Series, 2015, 635, 032013.	0.3	0
47	Dissociative dynamics of O₂ on Ag(110). Physical Chemistry Chemical Physics, 2015, 17, 9436-9445.	1.3	22
48	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
49	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
50	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
51	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
52	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
53	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
54	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 42 Td (stretchy="false">)</mml	2.9	27

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55	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
56	Electronic Friction Dominates Hydrogen Hot-Atom Relaxation on Pd(100). Physical Review Letters, 2014, 112, 103203.	2.9	112
57	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: 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
58	Energy-loss contribution to grazing scattering of fast He atoms from a silver surface. Physical Review A, 2014, 89, .	1.0	7
59	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
60	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
61	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 9779-9790.	1.5	20
62	Energy Dissipation Channels in Reactive and Non-reactive Scattering at Surfaces. Springer Series in Surface Sciences, 2013, , 371-388.	0.3	5
63	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
64	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
65	Diffusion of Hydrogen in Pd Assisted by Inelastic Ballistic Hot Electrons. Physical Review Letters, 2012, 108, 115902.	2.9	19
66	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
67	Dissociative and non-dissociative adsorption dynamics of N2 on Fe(110). Physical Chemistry Chemical Physics, 2012, 14, 7471.	1.3	37
68	Dynamics of Nitrogen Scattering off N-Covered Ag(111). Journal of Physical Chemistry C, 2012, 116, 21903-21912.	1.5	14
69	Energy dissipation channels in the adsorption of N on Ag(111). Computational and Theoretical Chemistry, 2012, 990, 126-131.	1.1	28
70	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
71	Electronic Stopping Power in Gold: The Role of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>Electrons and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">H</mml:mi><mml:mo>/</mml:mo><mml:mi>He</mml:mi></mml:math>Anomaly. Physical Review Letters, 2012, 108, 225504.	2.9	125
72	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

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73	JuaristietÂal.Reply:. Physical Review Letters, 2009, 102, .	2.9	28
74	Dissipative effects in the dynamics of N₂on tungsten surfaces. Journal of Physics Condensed Matter, 2009, 21, 264007.	0.7	30
75	LEIS: A reliable tool for surface composition analysis?. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 624-627.	0.6	12
76	Heating electrons with ion irradiation: A first-principles approach. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 590-593.	0.6	4
77	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
78	Energy-loss straggling of swift heavy ions in an electron gas. Physical Review A, 2008, 78, .	1.0	4
79	Crystal Effects in the Neutralization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>He</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>Ions in the Low Energy Ion Scattering Regime. Physical Review Letters, 2008, 100, 213201.	2.9	31
80	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
81	3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces. Physical Review A, 2007, 76, .	1.0	4
82	Electronic Stopping Power in LiF from First Principles. Physical Review Letters, 2007, 99, 235501.	2.9	157
83	Dynamic screening and electron dynamics in low-dimensional metal systems. Nuclear Instruments & Methods in Physics Research B, 2007, 258, 72-78.	0.6	8
84	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
85	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
86	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
87	Interaction of slow multicharged ions with surfaces. Radiation Physics and Chemistry, 2007, 76, 412-417.	1.4	4
88	Quantum-size effects in the energy loss of charged particles interacting with a confined two-dimensional electron gas. Physical Review A, 2006, 73, .	1.0	8
89	Energy loss of ions interacting with metal surfaces. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 148-157.	0.6	4
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	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
92	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
93	Spin-dependent electron emission from metals in the neutralization ofHe+ions. Physical Review A, 2005, 72, .	1.0	14
94	Band-structure-based collisional model for electronic excitations in ion-surface collisions. Physical Review A, 2005, 72, .	1.0	6
95	Transport cross sections based on a screened interaction potential: Comparison of classical and quantum-mechanical results. Physical Review A, 2005, 71, .	1.0	6
96	Spin-resolved pair-distribution functions in an electron gas: A scattering approach based on consistent potentials. Physical Review B, 2004, 69, .	1.1	9
97	Spin-dependent screening and Auger neutralization ofHe+ions in metals. Physical Review A, 2004, 70, .	1.0	27
98	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
99	Time-dependent screening in a two-dimensional electron gas. Surface Science, 2004, 559, 233-240.	0.8	9
100	Energy Loss in the Interaction of Atomic Particles with Solid Surfaces. Advances in Quantum Chemistry, 2004, , 223-245.	0.4	4
101	Molecular projectile effects for kinetic electron emission from carbon- and metal-surfaces bombarded by slow hydrogen ions. Nuclear Instruments & Methods in Physics Research B, 2003, 203, 1-7.	0.6	4
102	Ion induced electronic excitations in a spin-polarized electron gas. Nuclear Instruments & Methods in Physics Research B, 2003, 203, 83-88.	0.6	2
103	Time-dependent image potential at a metal surface. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 105-109.	0.8	9
104	Relaxation rate of excited electrons in an electron gas. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 117-126.	0.8	2
105	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
106	Charge-state dependence of kinetic electron emission induced by slow ions in metals. Physical Review A, 2003, 68, .	1.0	8
107	Energy loss of ions at metal surfaces: Band-structure effects. Physical Review A, 2003, 67, .	1.0	27
108	Energy loss of slow ions in a nonuniform electron gas. Physical Review B, 2003, 67, .	1.1	55

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109	Trajectory straggling and nonlinear effects in the energy loss of surface-channeled ions. Physical Review B, 2003, 67, .	1.1	9
110	Short-range correlation in an electron gas: A scattering approach. Physical Review B, 2003, 67, .	1.1	15
111	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
112	Nonlinear effects in the energy loss of a slow dipole in a free-electron gas. Physical Review A, 2002, 66, .	1.0	5
113	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
114	Channeling effects observed in energy-loss spectra of nitrogen ions scattered off a Pt(110) surface. Physical Review A, 2001, 64, .	1.0	35
115	Electronic stopping power ofAl2O3andSiO2for H, He, and N. Physical Review A, 2001, 64, .	1.0	22
116	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
117	Unexpected Behavior of the Stopping of Slow Ions in Ionic Crystals. Physical Review Letters, 2000, 84, 2124-2127.	2.9	56
118	Relaxation rate of excited electrons in metals: A nonperturbative calculation based on kinetic theory. Physical Review B, 2000, 63, .	1.1	10
119	Consistent model for the screening of slow muons in metals. Physical Review B, 1999, 60, R12546-R12548.	1.1	5
120	Charge State Dependence of the Energy Loss of Slow Ions in Metals. Physical Review Letters, 1999, 82, 1048-1051.	2.9	77
121	Energy loss of fast protons specularly reflected from metal surfaces. Nuclear Instruments & Methods in Physics Research B, 1999, 157, 104-109.	0.6	12
122	Charge state dependence of the energy loss of slow nitrogen ions reflected from an aluminum surface under grazing incidence. Nuclear Instruments & Methods in Physics Research B, 1999, 157, 87-91.	0.6	19
123	Atomic number dependence of the forward/backward kinetic electron emission induced by slow ions in carbon foils. Nuclear Instruments & Methods in Physics Research B, 1999, 157, 254-258.	0.6	4
124	Nonlinear effects in the kinetic electron emission induced by slow ions in metals. Nuclear Instruments & Methods in Physics Research B, 1998, 135, 487-491.	0.6	8
125	Coulomb explosion of H2+ in surface scattering. Nuclear Instruments & Methods in Physics Research B, 1998, 142, 473-485.	0.6	3
126	Contribution of the excitation of conduction band electrons to the kinetic electron emission induced by slow ions in metals. Physical Review B, 1998, 58, 15838-15846.	1.1	18

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127	Projectile charge dependence of kinetic electron emission from clean gold. Physica Scripta, 1997, T73, 322-323.	1.2	8
128	Interaction of multiply charged ions with metals. Nuclear Instruments & Methods in Physics Research B, 1996, 115, 173-176.	0.6	15
129	Energy loss of MeV protons specularly reflected from metal surfaces. Physical Review B, 1996, 53, 13839-13850.	1.1	37
130	Auger deexcitation rates in grazing atom-surface collisions. Nuclear Instruments & Methods in Physics Research B, 1995, 98, 424-428.	0.6	1
131	Nonlinear screening effects in the interaction of slow multicharged ions with metal surfaces. Nuclear Instruments & Methods in Physics Research B, 1995, 100, 279-283.	0.6	28
132	On the metallization of the LiF monolayer. Solid State Communications, 1994, 91, 957-960.	0.9	1
133	Energy loss in grazing proton-surface collisions. Nuclear Instruments & Methods in Physics Research B, 1994, 90, 252-256.	0.6	9
134	Charge transfer rates for excited states of protons at surfaces. Radiation Effects and Defects in Solids, 1994, null, 167-173.	0.4	1