Cristina Diaz

List of Publications by Year in descending order

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88 papers	2,351 citations	257357 24 h-index	223716 46 g-index
88 all docs	88 docs citations	88 times ranked	1692 citing authors

#	Article	IF	Citations
1	A simple model to engineer single-molecule conductance of acenes by chemical disubstitution. Nanoscale, 2022, 14, 464-472.	2.8	2
2	Grazing incidence fast atom and molecule diffraction: theoretical challenges. Physical Chemistry Chemical Physics, 2022, 24, 15628-15656.	1.3	3
3	Singleâ€Molecule Conductance of 1,4â€Azaborine Derivatives as Models of BNâ€doped PAHs. Angewandte Chemie - International Edition, 2021, 60, 6609-6616.	7.2	20
4	Normal and off-normal incidence dissociative dynamics of O₂(v,J) on ultrathin Cu films grown on Ru(0001). Physical Chemistry Chemical Physics, 2021, 23, 7768-7776.	1.3	0
5	Efficient photogeneration of nonacene on nanostructured graphene. Nanoscale Horizons, 2021, 6, 744-750.	4.1	9
6	Evaluation of the role of graphene-based Cu(<scp>i</scp>) catalysts in borylation reactions. Catalysis Science and Technology, 2021, 11, 3501-3513.	2.1	8
7	Theoretical study of structural and electronic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml -phase transition metal dichalcogenides. Physical Review B, 2021, 103, .	1.7	17
8	Defect formation in a graphene overlayer on ruthenium under high pressure. Physical Review B, 2020, 102, .	1.1	0
9	Accurate simulations of atomic diffractive scattering from KCl(0 0 1) under fast grazing incidence conditions. Nuclear Instruments & Methods in Physics Research B, 2020, 476, 1-9.	0.6	5
10	Prominent out-of-plane diffraction in helium scattering from a methyl-terminated Si(111) surface. Physical Chemistry Chemical Physics, 2019, 21, 15879-15887.	1.3	2
11	Tunable Graphene Electronics with Local Ultrahigh Pressure. Advanced Functional Materials, 2019, 29, 1806715.	7.8	15
12	Quantum Stereodynamics of H₂ Scattering from Co(0001): Influence of Reaction Channels. Journal of Physical Chemistry C, 2019, 123, 16223-16231.	1.5	8
13	Nonadiabatic scattering of NO off Au₃ clusters: A simple and robust diabatic state manifold generation method for multiconfigurational wavefunctions. Journal of Computational Chemistry, 2019, 40, 794-810.	1.5	10
14	Performance of van der Waals DFT approaches for helium diffraction on metal surfaces. Journal of Physics Condensed Matter, 2019, 31, 135901.	0.7	4
15	Electronic Properties of Sulfur Covered Ru(0001) Surfaces. Journal of Physical Chemistry A, 2018, 122, 2232-2240.	1.1	2
16	Molecular Modelling of the H₂â€Adsorptive Properties of Tetrazolateâ€Based Metalâ"Organic Frameworks: From the Cluster Approach to Periodic Simulations. ChemPhysChem, 2018, 19, 1349-1357.	1.0	6
17	Coverage evolution of the unoccupied Density of States in sulfur superstructures on Ru(0001). Applied Surface Science, 2018, 433, 300-305.	3.1	3
18	Graphene catalyzes the reversible formation of a Câ€"C bond between two molecules. Science Advances, 2018, 4, eaau9366.	4.7	9

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19	Theoretical Aspects of Hydrogen Dynamics at Metal Surfaces. , 2018, , 281-291.		0
20	Thickness-Dependent Reactivity of O₂ on Cu Layers Grown on Ru(0001) Surfaces. Journal of Physical Chemistry C, 2018, 122, 15529-15538.	1.5	8
21	Including London Dispersion Forces in Density Functional Theory (DFT + D): Applications to Molecule(Atom)/Surface Phenomena. , 2018, , 1-9.		0
22	Exploring surface landscapes with molecules: rotationally induced diffraction of H₂ on LiF(001) under fast grazing incidence conditions. Physical Chemistry Chemical Physics, 2017, 19, 16317-16322.	1.3	8
23	Dissociative and non-dissociative adsorption of O₂ on Cu(111) and Cu_{ML}/Ru(0001) surfaces: adiabaticity takes over. Physical Chemistry Chemical Physics, 2017, 19, 10217-10221.	1.3	20
24	A DFT study of Cu nanoparticles adsorbed on defective graphene. Applied Surface Science, 2017, 412, 146-151.	3.1	20
25	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>LiF</mml:mi><mml:mrow> diffractive scattering under fast grazing incidence using a DFT-based potential energy surface. Physical Review B, 2017, 96, .	1.1	7
26	Experimental and theoretical study of rotationally inelastic diffraction of H2(D2) from methyl-terminated Si(111). Journal of Chemical Physics, 2016, 145, 084705.	1.2	3
27	Diffraction of H from LiF(001): From slow normal incidence to fast grazing incidence. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 49-53.	0.6	22
28	Understanding the self-assembly of TCNQ on Cu(111): a combined study based on scanning tunnelling microscopy experiments and density functional theory simulations. RSC Advances, 2016, 6, 15071-15079.	1.7	22
29	Role of van der Waals forces in the diffraction of noble gases from metal surfaces. Physical Review B, 2016, 93, .	1.1	21
30	Enigmatic HCl + Au(111) Reaction: A Puzzle for Theory and Experiment. Journal of Physical Chemistry C, 2016, 120, 25760-25779.	1.5	48
31	Quantum and classical dynamics of reactive scattering of H₂ from metal surfaces. Chemical Society Reviews, 2016, 45, 3658-3700.	18.7	137
32	XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015). Journal of Physics: Conference Series, 2015, 635, 001001.	0.3	0
33	Understanding the rotational excitation in scattering of D₂ from CH₃-Si(111). Journal of Physics: Conference Series, 2015, 635, 032007.	0.3	0
34	Theoretical study of noble gases diffraction from Ru(0001) using van der Waals DFT-based potentials. Journal of Physics: Conference Series, 2015, 635, 032004.	0.3	0
35	The role of the initial ro-vibrational state in molecule/surface scattering under fast grazing incidence. Journal of Physics: Conference Series, 2015, 635, 012029.	0.3	1
36	Six-dimensional theoretical study of H₂scattering from LiF(001): From thermal to high incidence energies. Journal of Physics: Conference Series, 2015, 635, 032012.	0.3	0

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37	Scattering of H(D) from LiF(100) under fast grazing incidence conditions: To what extent is classical dynamics a useful tool?. Nuclear Instruments & Methods in Physics Research B, 2015, 354, 9-15.	0.6	9
38	Assessing the reliability of van der Waals DFT functionals to study the physisorption of molecular hydrogen on aromatic systems. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	6
39	Theoretical Simulations of Reactive and Nonreactive Scattering of Light Diatomic Molecules from Metal Surfaces: Past, Present, and Future. Advances in Chemistry, 2014, 2014, 1-21.	1.1	0
40	Dissociation and recombination of D2 on Cu(111): Ab initio molecular dynamics calculations and improved analysis of desorption experiments. Journal of Chemical Physics, 2014, 141, 124705.	1.2	35
41	Controlling the spatial arrangement of organic magnetic anions adsorbed on epitaxial graphene on Ru(0001). Nanoscale, 2014, 6, 15271-15279.	2.8	19
42	Probing the Site-Dependent Kondo Response of Nanostructured Graphene with Organic Molecules. Nano Letters, 2014, 14, 4560-4567.	4.5	24
43	Environment-driven reactivity of H2 on PdRu surface alloys. Physical Chemistry Chemical Physics, 2013, 15, 14936.	1.3	15
44	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	1.1	35
45	Elastic Response of Graphene Nanodomes. ACS Nano, 2013, 7, 2927-2934.	7.3	35
46	Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene. Nature Physics, 2013, 9, 368-374.	6.5	158
47	Ordered arrays of metalâ€“organic magnets at surfaces. Journal of Physics Condensed Matter, 2013, 25, 484007.	0.7	16
48	Thermal Lattice Expansion Effect on Reactive Scattering of H₂ from Cu(111) at T_s = 925 K. Journal of Physical Chemistry A, 2013, 117, 8770-8781.	1.1	50
49	Using Molecular Reflectivity to Explore Reaction Dynamics at Metal Surfaces. Springer Series in Surface Sciences, 2013, , 75-100.	0.3	2
50	Helium, neon and argon diffraction from Ru(0001). Journal of Physics Condensed Matter, 2012, 24, 354002.	0.7	16
51	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
52	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	1.1	34
53	Reactive scattering of H₂ (Î½ â‰¥ 0,Jâ‰¥ 0) from metal surfaces under fast-grazing incidence conditions. Journal of Physics: Conference Series, 2012, 388, 132005.	0.3	0
54	Dynamics of H2 dissociation on the 1/2 ML c(2 Ã— 2)-Ti/Al(100) surface. Physical Chemistry Chemical Physics, 2012, 14, 3234.	1.3	14

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55	H₂ Diffraction from a Strained Pseudomorphic Monolayer of Cu Deposited on Ru(0001). Journal of Physical Chemistry C, 2012, 116, 13671-13678.	1.5	15
56	Effect of Surface Motion on the Rotational Quadrupole Alignment Parameter of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">D</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Reacting on Cu(111). Physical Review Letters, 2012, 108, 236104.	2.9	95
57	Hydrogen dissociation on Cu(111): the influence of lattice motion. Part I. Physical Chemistry Chemical Physics, 2011, 13, 4552.	1.3	53
58	A density functional theory study of the manganese-phthalocyanine. Theoretical Chemistry Accounts, 2011, 128, 497-503.	0.5	30
59	Six-dimensional quasiclassical and quantum dynamics of H2 dissociation on the c(2 Ã— 2)-Ti/Al(100) surface. Journal of Chemical Physics, 2011, 134, 114708.	1.2	13
60	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	2.9	129
61	Grazing incidence scattering of vibrationally excited H2 molecules from metal surfaces. Surface Science, 2010, 604, 2031-2035.	0.8	8
62	Reactive scattering of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>from metal surfaces under fast-grazing-incidence conditions. Physical Review A, 2010, 82, .	1.0	10
63	Nonmonotonic dissociative adsorption of vibrationally excited<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>metal surfaces. Physical Review B, 2010, 81, .	1.1	12
64	Apparent failure of the Bornâ€“Oppenheimer static surface model for vibrational excitation of molecular hydrogen on copper. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20881-20886.	3.3	46
65	Dynamics on Six-Dimensional Potential Energy Surfaces for H₂/Cu(111): Corrugation Reducing Procedure versus Modified Shepard Interpolation Method and PW91 versus RPBE. Journal of Physical Chemistry C, 2010, 114, 11192-11201.	1.5	53
66	Experimental and theoretical study of rotationally inelastic diffraction of D2 from NiAl(110). Physical Chemistry Chemical Physics, 2010, 12, 14501.	1.3	11
67	Six-dimensional dynamics study of reactive and non reactive scattering of H2 from Cu(111) using a chemically accurate potential energy surface. Physical Chemistry Chemical Physics, 2010, 12, 6499.	1.3	88
68	Dynamics of dissociative adsorption of hydrogen on a CO-precovered Ru(0001) surface: a comparison of theoretical and experimental results. Physical Chemistry Chemical Physics, 2010, 12, 1331-1340.	1.3	17
69	Molecular Effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Scattering from Metal Surfaces at Grazing Incidence. Physical Review Letters, 2009, 103, 013201.	2.9	21
70	A note on the vibrational efficacy in molecule-surface reactions. Journal of Chemical Physics, 2009, 130, 094706.	1.2	25
71	Chemically Accurate Simulation of a Prototypical Surface Reaction: H ₂ Dissociation on Cu(111). Science, 2009, 326, 832-834.	6.0	315
72	Molecular effects in grazing incidence collisions of H₂with metal surfaces. Journal of Physics: Conference Series, 2009, 194, 012058.	0.3	0

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73	Associative desorption of N2 from Ru(0001): A computational study. Chemical Physics Letters, 2007, 434, 231-236.	1.2	23
74	Reactive and nonreactive scattering of N2 from Ru(0001): A six-dimensional adiabatic study. Journal of Chemical Physics, 2006, 125, 114706.	1.2	43
75	Experimental evidence of dynamic trapping in the scattering of H2 from Pd(110). Journal of Chemical Physics, 2006, 125, 051101.	1.2	16
76	Multidimensional Effects on Dissociation ofN2on Ru(0001). Physical Review Letters, 2006, 96, 096102.	2.9	89
77	DYNAMICS OF H₂ CHEMISORPTION ON METAL SURFACES. , 2006, , .		0
78	Quantum and classical dynamics ofH2scattering from Pd(111) at off-normal incidence. Physical Review B, 2005, 72, .	1.1	22
79	A classical dynamics method for H2 diffraction from metal surfaces. Journal of Chemical Physics, 2005, 122, 154706.	1.2	28
80	In-Plane and Out-of-Plane Diffraction ofH2from Metal Surfaces. Physical Review Letters, 2004, 93, 246104.	2.9	72
81	Theoretical analysis of the relation between H2 dissociation and reflection on Pd surfaces. Journal of Chemical Physics, 2004, 120, 321-328.	1.2	23
82	Pronounced out-of-plane diffraction of H2 molecules from a Pd(111) surface. Chemical Physics Letters, 2004, 390, 250-255.	1.2	55
83	Theoretical and Experimental Study of the Scattering of H2 from Pd(111). Physica Scripta, 2004, 110, 394.	1.2	5
84	Angular distribution of H[sub 2] molecules scattered from the Pd(111) surface. Journal of Chemical Physics, 2003, 118, 2886.	1.2	30
85	Time-dependent close-coupling calculations of double ionization of helium by protons and antiprotons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 2555-2566.	0.6	15
86	Double ionization of He by antiproton impact using a convergent frozen-correlation approximation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, L403-L409.	0.6	9
87	The role of dynamic correlation in double ionization of He by high-energy protons and antiprotons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 4373-4388.	0.6	15
88	7D Quantum Dynamics of H₂Scattering from Cu(111): The Accuracy of the Phonon Sudden Approximation. Zeitschrift Fur Physikalische Chemie, 0, , 130617035227002.	1.4	17