Ye Xu

List of Publications by Year in descending order

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130	13,981	38660	20307
papers	citations	h-index	g-index
137	137	137	13543
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	Singleâ€Junction Organic Photovoltaic Cells with Approaching 18% Efficiency. Advanced Materials, 2020, 32, e1908205.	11.1	1,407
2	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	3.1	1,167
3	On the origin of the catalytic activity of gold nanoparticles for low-temperature CO oxidation. Journal of Catalysis, 2004, 223, 232-235.	3.1	1,122
4	Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates. Angewandte Chemie - International Edition, 2005, 44, 2132-2135.	7.2	1,015
5	Adsorption and Dissociation of O2on Ptâ^'Co and Ptâ^'Fe Alloys. Journal of the American Chemical Society, 2004, 126, 4717-4725.	6.6	615
6	Catalytically active Au-O(OH) $\langle i \rangle \langle sub \rangle \times \langle sub \rangle \langle i \rangle$ - species stabilized by alkali ions on zeolites and mesoporous oxides. Science, 2014, 346, 1498-1501.	6.0	544
7	Ecoâ€Compatible Solventâ€Processed Organic Photovoltaic Cells with Over 16% Efficiency. Advanced Materials, 2019, 31, e1903441.	11.1	445
8	Wide-gap non-fullerene acceptor enabling high-performance organic photovoltaic cells for indoor applications. Nature Energy, 2019, 4, 768-775.	19.8	407
9	Achieving Over 15% Efficiency in Organic Photovoltaic Cells via Copolymer Design. Advanced Materials, 2019, 31, e1808356.	11.1	388
10	14.7% Efficiency Organic Photovoltaic Cells Enabled by Active Materials with a Large Electrostatic Potential Difference. Journal of the American Chemical Society, 2019, 141, 7743-7750.	6.6	379
11	Adsorption and Dissociation of O2on Gold Surfaces:Â Effect of Steps and Strain. Journal of Physical Chemistry B, 2003, 107, 9298-9307.	1.2	322
12	Pd–Ir Core–Shell Nanocubes: A Type of Highly Efficient and Versatile Peroxidase Mimic. ACS Nano, 2015, 9, 9994-10004.	7. 3	254
13	Atomic and molecular adsorption on Pt(111). Surface Science, 2005, 587, 159-174.	0.8	247
14	Bimetallic and Ternary Alloys for Improved Oxygen Reduction Catalysis. Topics in Catalysis, 2007, 46, 276-284.	1.3	202
15	Defect engineering activating (Boosting) zinc storage capacity of MoS2. Energy Storage Materials, 2019, 16, 527-534.	9.5	199
16	Recent Progress in Chlorinated Organic Photovoltaic Materials. Accounts of Chemical Research, 2020, 53, 822-832.	7.6	198
17	Partial and complete reduction of O2 by hydrogen on transition metal surfaces. Surface Science, 2010, 604, 1565-1575.	0.8	189
18	Adsorption and dissociation of O2 on Cu(): thermochemistry, reaction barrier and the effect of strain. Surface Science, 2001, 494, 131-144.	0.8	175

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19	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111). Journal of Physical Chemistry C, 2008, 112, 9559-9572.	1.5	173
20	Reversibility of Noble Metal-Catalyzed Aprotic Li-O ₂ Batteries. Nano Letters, 2015, 15, 8084-8090.	4.5	165
21	Effect of Subsurface Oxygen on the Reactivity of the Ag(111) Surface. Journal of the American Chemical Society, 2005, 127, 12823-12827.	6.6	151
22	Potential-Dependent Generation of O ₂ ^{â€"} and LiO ₂ and Their Critical Roles in O ₂ Reduction to Li ₂ O ₂ in Aprotic Liâ€"O ₂ Batteries. Journal of Physical Chemistry C, 2016, 120, 3690-3698.	1,5	149
23	Tuning the Hybridization of Local Exciton and Chargeâ€Transfer States in Highly Efficient Organic Photovoltaic Cells. Angewandte Chemie - International Edition, 2020, 59, 9004-9010.	7.2	144
24	Amorphous Li ₂ O ₂ : Chemical Synthesis and Electrochemical Properties. Angewandte Chemie - International Edition, 2016, 55, 10717-10721.	7.2	135
25	A New Conjugated Polymer that Enables the Integration of Photovoltaic and Lightâ€Emitting Functions in One Device. Advanced Materials, 2021, 33, e2101090.	11.1	129
26	Aqueousâ€Phase Hydrogenation of Acetic Acid over Transition Metal Catalysts. ChemCatChem, 2010, 2, 1420-1424.	1.8	123
27	Rational Anode Engineering Enables Progresses for Different Types of Organic Solar Cells. Advanced Energy Materials, 2021, 11, 2100492.	10.2	108
28	Thermoplastic Elastomer Tunes Phase Structure and Promotes Stretchability of Highâ€Efficiency Organic Solar Cells. Advanced Materials, 2021, 33, e2106732.	11.1	101
29	Enhanced π–π Interactions of Nonfullerene Acceptors by Volatilizable Solid Additives in Efficient Polymer Solar Cells. Advanced Materials, 2019, 31, e1900477.	11.1	99
30	Oxygen Vacancy-Assisted Coupling and Enolization of Acetaldehyde on CeO ₂ (111). Journal of the American Chemical Society, 2012, 134, 18034-18045.	6.6	97
31	Lattice strain effects on CO oxidation on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 3369.	1.3	96
32	O 2 reduction by lithium on Au(111) and Pt(111). Journal of Chemical Physics, 2010, 133, 024703.	1.2	88
33	Strain Effect in Palladium Nanostructures as Nanozymes. Nano Letters, 2020, 20, 272-277.	4.5	85
34	DFT-Based Method for More Accurate Adsorption Energies: An Adaptive Sum of Energies from RPBE and vdW Density Functionals. Journal of Physical Chemistry C, 2017, 121, 4937-4945.	1.5	80
35	High-throughput screening of monometallic catalysts for aqueous-phase hydrogenation of biomass-derived oxygenates. Applied Catalysis B: Environmental, 2013, 140-141, 98-107.	10.8	78
36	Direct Detection of the Superoxide Anion as a Stable Intermediate in the Electroreduction of Oxygen in a Nonâ€Aqueous Electrolyte Containing Phenol as a Proton Source. Angewandte Chemie - International Edition, 2015, 54, 8165-8168.	7.2	78

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37	Effect of Particle Size on the Oxidizability of Platinum Clusters. Journal of Physical Chemistry A, 2006, 110, 5839-5846.	1.1	75
38	Trends in the Catalytic Activity of Transition Metals for the Oxygen Reduction Reaction by Lithium. Journal of Physical Chemistry Letters, 2012, 3, 891-895.	2.1	75
39	Reduced Nonradiative Energy Loss Caused by Aggregation of Nonfullerene Acceptor in Organic Solar Cells. Advanced Energy Materials, 2019, 9, 1901823.	10.2	72
40	Printable MoO <i></i> Anode Interlayers for Organic Solar Cells. Advanced Materials, 2018, 30, e1801718.	11.1	71
41	A Highâ€Performance Nonfused Wideâ€Bandgap Acceptor for Versatile Photovoltaic Applications. Advanced Materials, 2022, 34, e2108090.	11.1	71
42	Molecular design revitalizes the low-cost PTV-polymer for highly efficient organic solar cells. National Science Review, 2021, 8, nwab031.	4.6	70
43	Adsorption and dissociation of O2 on Ir(111). Journal of Chemical Physics, 2002, 116, 10846-10853.	1.2	67
44	Oxygen Reduction by Lithium on Model Carbon and Oxidized Carbon Structures. Journal of the Electrochemical Society, 2011, 158, A1177.	1.3	66
45	Low Temperature Aggregation Transitions in N3 and Y6 Acceptors Enable Doubleâ€Annealing Method That Yields Hierarchical Morphology and Superior Efficiency in Nonfullerene Organic Solar Cells. Advanced Functional Materials, 2020, 30, 2005011.	7.8	66
46	Unlocking the energy capabilities of micron-sized LiFePO4. Nature Communications, 2015, 6, 7898.	5.8	65
47	Temperature evolution of structure and bonding of formic acid and formate on fully oxidized and highly reduced CeO2(111). Physical Chemistry Chemical Physics, 2009, 11, 11171.	1.3	61
48	Impact of Electrostatic Interaction on Bulk Morphology in Efficient Donor–Acceptor Photovoltaic Blends. Angewandte Chemie - International Edition, 2021, 60, 15988-15994.	7.2	60
49	Identifying Active Functionalities on Fewâ€Layered Graphene Catalysts for Oxidative Dehydrogenation of Isobutane. ChemSusChem, 2014, 7, 483-491.	3.6	56
50	Quadrupole Moment Induced Morphology Control Via a Highly Volatile Small Molecule in Efficient Organic Solar Cells. Advanced Functional Materials, 2021, 31, 2010535.	7.8	55
51	Thermodynamic Equilibrium Compositions, Structures, and Reaction Energies of PtxOy(x= 1â^'3) Clusters Predicted from First Principles. Journal of Physical Chemistry B, 2006, 110, 16591-16599.	1.2	51
52	Effects of hydrogen and water on the activity and selectivity of acetic acid hydrogenation on ruthenium. Green Chemistry, 2014, 16, 911-924.	4.6	49
53	The adsorption and dissociation of O 2 molecular precursors on Cu: the effect of steps. Surface Science, 2003, 538, 219-232.	0.8	47
54	Multi-component non-fullerene acceptors with tunable bandgap structures for efficient organic solar cells. Journal of Materials Chemistry A, 2018, 6, 23644-23649.	5.2	47

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55	Bioalcohol production from acidogenic products via a two-step process: A case study of butyric acid to butanol. Applied Energy, 2019, 252, 113482.	5.1	47
56	Recent Advances in Fullereneâ€free Polymer Solar Cells: Materials and Devices. Chinese Journal of Chemistry, 2019, 37, 207-215.	2.6	46
57	A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics. Physical Chemistry Chemical Physics, 2008, 10, 6009.	1.3	45
58	Reactivity and reaction intermediates for acetic acid adsorbed on CeO2(1 1 1). Catalysis Today, 2015, 253, 65-76.	2.2	43
59	Efficient charge generation at low energy losses in organic solar cells: a key issues review. Reports on Progress in Physics, 2020, 83, 082601.	8.1	43
60	Recent progress in reducing voltage loss in organic photovoltaic cells. Materials Chemistry Frontiers, 2021, 5, 709-722.	3.2	41
61	Mapping the energy level alignment at donor/acceptor interfaces in non-fullerene organic solar cells. Nature Communications, 2022, 13, 2046.	5.8	41
62	Exploring the structure and chemical activity of 2-D gold islands on graphene moir \tilde{A} \mathbb{Q} /Ru(0001). Faraday Discussions, 2011, 152, 267.	1.6	37
63	Amorphous Li ₂ O ₂ : Chemical Synthesis and Electrochemical Properties. Angewandte Chemie, 2016, 128, 10875-10879.	1.6	37
64	Simultaneous Improvement of Efficiency and Stability of Organic Photovoltaic Cells by using a Crossâ€Linkable Fullerene Derivative. Small, 2021, 17, e2101133.	5.2	34
65	Organic photovoltaic cells with high efficiencies for both indoor and outdoor applications. Materials Chemistry Frontiers, 2021, 5, 893-900.	3.2	32
66	Oxygen electrochemistry in Liâ€O ₂ batteries probed by in situ surfaceâ€enhanced Raman spectroscopy. SusMat, 2021, 1, 345-358.	7.8	31
67	The effect of aggregation behavior on photovoltaic performances in benzodithiophene-thiazolothiazole-based wide band-gap conjugated polymers with side chain position changes. Polymer Chemistry, 2020, 11, 1629-1636.	1.9	30
68	Formation and stability of dense arrays of Au nanoclusters on hexagonal boron nitride/Rh(111). Physical Review B, 2014, 89, .	1.1	29
69	Adsorption of Propane, Isopropyl, and Hydrogen on Cluster Models of the M1 Phase of Moâ^'Vâ^'Teâ^'Nbâ^'O Mixed Metal Oxide Catalyst. Journal of Physical Chemistry C, 2010, 114, 4544-4549.	1.5	28
70	Adsorption and Diffusion of 4d and 5d Transition Metal Adatoms on Graphene/Ru(0001) and the Implications for Cluster Nucleation. Topics in Catalysis, 2014, 57, 69-79.	1.3	28
71	p-Doped Conducting Polyelectrolyte as an Anode Interlayer Enables High Efficiency for 1 cm $<$ sup $>$ 2 $<$ /sup $>$ Printed Organic Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 20205-20213.	4.0	28
72	CO Adsorption on Au Nanoparticles Grown on Hexagonal Boron Nitride/Rh(111). Journal of Physical Chemistry C, 2016, 120, 10909-10918.	1.5	27

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73	CoCrFeNi High-Entropy Alloy as an Enhanced Hydrogen Evolution Catalyst in an Acidic Solution. Journal of Physical Chemistry C, 2021, 125, 17008-17018.	1.5	25
74	Propane Ammoxidation Over the Mo–V–Te–Nb–O M1 Phase: Reactivity of Surface Cations in Hydrogen Abstraction Steps. Topics in Catalysis, 2011, 54, 605-613.	1.3	24
7 5	Mechanistic origin of low polarization in aprotic Na–O ₂ batteries. Physical Chemistry Chemical Physics, 2017, 19, 12375-12383.	1.3	24
76	Enhancing the Photovoltaic Performance of Nonfullerene Acceptors via Conjugated Rotatable End Groups. Advanced Energy Materials, 2018, 8, 1802131.	10.2	24
77	Investigating the Trade-Off between Device Performance and Energy Loss in Nonfullerene Organic Solar Cells. ACS Applied Materials & Solar Cells.	4.0	24
78	Tuning the Hybridization of Local Exciton and Chargeâ€Transfer States in Highly Efficient Organic Photovoltaic Cells. Angewandte Chemie, 2020, 132, 9089-9095.	1.6	24
79	Activation of methyl acetate on Pd(111). Surface Science, 2010, 604, 887-892.	0.8	23
80	Coupling of Acetaldehyde to Crotonaldehyde on CeO _{2â€"<i>x</i>} (111): Bifunctional Mechanism and Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2019, 123, 8273-8286.	1.5	23
81	Adsorption and diffusion of the Rh and Au adatom on graphene moiré/Ru(0001). Journal of Chemical Physics, 2013, 138, 184710.	1.2	22
82	Adsorption Energy of <i>tert</i> -Butyl on Pt(111) by Dissociation of <i>tert</i> -Butyl lodide: Calorimetry and DFT. Journal of Physical Chemistry C, 2014, 118, 427-438.	1.5	22
83	CO ₂ electrochemical reduction at thiolate-modified bulk Au electrodes. Catalysis Science and Technology, 2019, 9, 2689-2701.	2.1	22
84	Propane ammoxidation over Mo–V–Te–Nb–O M1 phase: Density functional theory study of propane oxidative dehydrogenation steps. Catalysis Today, 2014, 238, 28-34.	2.2	21
85	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. Journal of Physical Chemistry C, 2014, 118, 20043-20069.	1.5	21
86	Significant Effect of Fluorination on Simultaneously Improving Work Function and Transparency of Anode Interlayer for Organic Solar Cells. Advanced Energy Materials, 2019, 9, 1803826.	10.2	21
87	A combined HAADF STEM and density functional theory study of tantalum and niobium locations in the Mo–V–Te–Ta(Nb)–O M1 phases. Catalysis Communications, 2012, 29, 68-72.	1.6	19
88	Direct Detection of the Superoxide Anion as a Stable Intermediate in the Electroreduction of Oxygen in a Nonâ€Aqueous Electrolyte Containing Phenol as a Proton Source. Angewandte Chemie, 2015, 127, 8283-8286.	1.6	19
89	Efficient Exciton Dissociation Enabled by the End Group Modification in Non-Fullerene Acceptors. Journal of Physical Chemistry C, 2020, 124, 7691-7698.	1.5	18
90	Effect of Pd surface structure on the activation of methyl acetate. Catalysis Today, 2011, 165, 96-105.	2.2	17

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91	Graphene moir \tilde{A} © structure grown on a pseudomorphic metal overlayer supported on Ru(0001). Surface Science, 2013, 611, 67-73.	0.8	17
92	Theoretical investigation of dephosphorylation of phosphate monoesters on CeO2(111). Catalysis Today, 2018, 312, 141-148.	2.2	16
93	Squaraine organic crystals with strong dipole effect toward stable lithium-organic batteries. Energy Storage Materials, 2021, 41, 240-247.	9.5	16
94	Adsorption of transition metal adatoms on h-BN/Rh(111): Implications for nanocluster self-assembly. Catalysis Today, 2017, 280, 220-231.	2.2	15
95	Simulated Temperature Programmed Desorption of Acetaldehyde on CeO2(111): Evidence for the Role of Oxygen Vacancy and Hydrogen Transfer. Topics in Catalysis, 2017, 60, 446-458.	1.3	15
96	Spectroscopic Identification of the Au–C Bond Formation upon Electroreduction of an Aryl Diazonium Salt on Gold. Langmuir, 2016, 32, 11514-11519.	1.6	14
97	Quantifying $\langle i \rangle V \langle i \rangle \langle sub \rangle oc \langle sub \rangle$ loss induced by alkyl pendants of acceptors in organic solar cells. Journal of Materials Chemistry C, 2020, 8, 12568-12577.	2.7	14
98	Elucidating the Mechanism of Ambient-Temperature Aldol Condensation of Acetaldehyde on Ceria. ACS Catalysis, 2021, 11, 8621-8634.	5.5	14
99	Decomposition of Furan on Pd(111). Topics in Catalysis, 2012, 55, 290-299.	1.3	13
100	Energetics of Adsorbed CH ₂ and CH on Pt(111) by Calorimetry: The Dissociative Adsorption of Diiodomethane. Journal of Physical Chemistry C, 2014, 118, 29310-29321.	1.5	13
101	Covalent versus localized nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi>electrons in ceria: Resonant angle-resolved photoemission spectroscopy and density functional theory. Physical Review B, 2017, 95, .</mml:mrow></mml:math>	<td>ows</td>	ows
102	An experimental and theoretical study of adenine adsorption on Au(111). Physical Chemistry Chemical Physics, 2018, 20, 4688-4698.	1.3	13
103	The Effect of Coadsorbed Oxygen on the Adsorption and Diffusion of Potassium on Rh(110):  A First-Principles Study. Journal of Physical Chemistry C, 2007, 111, 7446-7455.	1.5	12
104	Design of ultra-high luminescent polymers for organic photovoltaic cells with low energy loss. Chemical Communications, 2021, 57, 9132-9135.	2.2	12
105	Propane Ammoxidation over Mo–V–Te–Nb–O M1 Phase Investigated by DFT: Elementary Steps of Ammonia Adsorption, Activation and NH Insertion into π-Allyl Intermediate. Topics in Catalysis, 2014, 57, 1145-1151.	1.3	11
106	Impact of Electrostatic Interaction on Bulk Morphology in Efficient Donor–Acceptor Photovoltaic Blends. Angewandte Chemie, 2021, 133, 16124-16130.	1.6	11
107	Recent Developments in the Electrocatalysis of the O2 Reduction Reaction. , 0, , 271-315.		10
108	Design of ultranarrow-bandgap acceptors for efficient organic photovoltaic cells and highly sensitive organic photodetectors. Journal of Energy Chemistry, 2022, 72, 388-394.	7.1	10

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109	Reconciling the electronic and geometric corrugations of the hexagonal boron nitride and graphene nanomeshes. Surface Science, 2015, 642, L16-L19.	0.8	9
110	Estimation of electric field effects on the adsorption of molecular superoxide species on Au based on density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 32626-32635.	1.3	8
111	Adsorption structure of adenine on cerium oxide. Applied Surface Science, 2020, 530, 147257.	3.1	8
112	Reduced Nonradiative Recombination Energy Loss Enabled Efficient Polymer Solar Cells via Tuning Alkyl Chain Positions on Pendent Benzene Units of Polymers. ACS Applied Materials & Samp; Interfaces, 2020, 12, 24184-24191.	4.0	7
113	Theoretical analysis of the adsorption of phosphoric acid and model phosphate monoesters on CeO2(111). Surface Science, 2021, 705, 121776.	0.8	6
114	Reaction pathways for HCN on transition metal surfaces. Physical Chemistry Chemical Physics, 2019, 21, 5274-5284.	1.3	4
115	Hydrogen Adsorption on Ordered and Disordered Pt-Ni Alloys. Topics in Catalysis, 2020, 63, 714-727.	1.3	4
116	Thermal stability and protective properties of phenylphosphonic acid on Cu(111). Applied Surface Science, 2022, 600, 154036.	3.1	1
117	Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity., 2006,, 289-309.		0
118	Efficiency enhancements of a restricted stochastic search algorithm for locating local and global minima. Chemical Physics Letters, 2019, 725, 1-7.	1.2	0
119	Catalytic Encounters at the Molecular Level: Gabor A. Somorjai Award Symposium for Creative Research in Catalysis in Honor of Professor Manos Mavrikakis. Topics in Catalysis, 2020, 63, 617-617.	1.3	0
120	Squaraine Organic Crystals with Strong Dipole Effect Toward Stable Lithium-Organic Batteries. SSRN Electronic Journal, 0, , .	0.4	0
121	Role of Superoxide Anion in the Oxygen Reduction Reaction in Non-Aqueous Electrolytes with a Proton or Lithium Source. ECS Meeting Abstracts, 2016, , .	0.0	0
122	Theoretical Investigation of the Oxygen Reduction Reaction in Non-Aqueous Electrolytes. ECS Meeting Abstracts, 2016, , .	0.0	0
123	Enhanced Electrocatalytic CO2 Reduction on Thiol-Functionalized Gold. ECS Meeting Abstracts, 2016, , .	0.0	0
124	Tuning the Selectivity of CO2 Electrochemical Reduction Toward Hydrocarbon with Ligand Modified Metal Electrocatalyst. ECS Meeting Abstracts, 2016, , .	0.0	0
125	Theoretical Investigation of Oxygen- and Bromine-Functionalized Model Carbon Structures for Li-Redox Activity. ECS Meeting Abstracts, 2017, , .	0.0	0
126	Hydrogenation at Metal-Ligand Interfaces in CO2 Electrochemical Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0

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127	Mechanistic Insights into Oxygen Reduction and Evolution Reactions in Non-Aqueous Metal-Air Batteries. ECS Meeting Abstracts, 2017, , .	0.0	O
128	Interaction of Thiol Ligands with Gold in Electrocatalytic CO2 Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0
129	Mechanistic Insights into Oxygen Reduction Reactions in Non-Aqueous Metal-Air Batteries. ECS Meeting Abstracts, 2018, , .	0.0	0
130	Theoretical Investigation of the Effects of Metal Cations on Oxygen Reduction Reaction in Non-Aqueous Li-Air Batteries. ECS Meeting Abstracts, 2019, , .	0.0	0