Ivan Infante

List of Publications by Year
in descending order

126 papers	7,993 citations	41344 49 h-index	53230 85 g-index
135 all docs	135 docs citations	135 times ranked	7987 citing authors

#	Article	IF	Citations
1	Colloidal CsPbX₃ (X = Cl, Br, I) Nanocrystals 2.0: Zwitterionic Capping Ligands for Improved Durability and Stability. ACS Energy Letters, 2018, 3, 641-646.	17.4	647
2	Rationalizing and Controlling the Surface Structure and Electronic Passivation of Cesium Lead Halide Nanocrystals. ACS Energy Letters, 2019, 4, 63-74.	17.4	308
3	The Chemical Bond between Au(I) and the Noble Gases. Comparative Study of NgAuF and NgAu⁺ (Ng = Ar, Kr, Xe) by Density Functional and Coupled Cluster Methods. Journal of the American Chemical Society, 2008, 130, 1048-1060.	13.7	260
4	Highly Emissive Selfâ€Trapped Excitons in Fully Inorganic Zeroâ€Dimensional Tin Halides. Angewandte Chemie - International Edition, 2018, 57, 11329-11333.	13.8	242
5	On the Origin of Surface Traps in Colloidal IIâ€“VI Semiconductor Nanocrystals. Chemistry of Materials, 2017, 29, 752-761.	6.7	231
6	Surface Traps in Colloidal Quantum Dots: A Combined Experimental and Theoretical Perspective. Journal of Physical Chemistry Letters, 2017, 8, 5209-5215.	4.6	231
7	Equilibrium Mercury Isotope Fractionation between Dissolved Hg(II) Species and Thiol-Bound Hg. Environmental Science & Technology, 2010, 44, 4191-4197.	10.0	230
8	Emissive Bi-Doped Double Perovskite Cs₂Ag_{1â€“<i>x</i>}Na_{<i>x</i>}InCl₆ Nanocrystals. ACS Energy Letters, 2019, 4, 1976-1982.	17.4	198
9	Surface Termination, Morphology, and Bright Photoluminescence of Cesium Lead Halide Perovskite Nanocrystals. ACS Energy Letters, 2016, 1, 1266-1272.	17.4	195
10	Simultaneous Cationic and Anionic Ligand Exchange For Colloidally Stable CsPbBr₃ Nanocrystals. ACS Energy Letters, 2019, 4, 819-824.	17.4	173
11	Finding and Fixing Traps in IIâ€“VI and IIIâ€“V Colloidal Quantum Dots: The Importance of Z-Type Ligand Passivation. Journal of the American Chemical Society, 2018, 140, 15712-15723.	13.7	166
12	â€œDarker-than-Blackâ€•PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands. Journal of the American Chemical Society, 2015, 137, 1875-1886.	13.7	149
13	Resurfacing halide perovskite nanocrystals. Science, 2019, 364, 833-834.	12.6	143
14	Unexpected trends in halogen-bond based noncovalent adducts. Chemical Communications, 2012, 48, 7708.	4.1	136
15	On the directionality of halogen bonding. Physical Chemistry Chemical Physics, 2013, 15, 10350.	2.8	136
16	The Phosphine Oxide Route toward Lead Halide Perovskite Nanocrystals. Journal of the American Chemical Society, 2018, 140, 14878-14886.	13.7	136
17	Shape-Pure, Nearly Monodispersed CsPbBr₃ Nanocubes Prepared Using Secondary Aliphatic Amines. Nano Letters, 2018, 18, 7822-7831.	9.1	132
18	Colloidal CdSe Nanoplatelets, A Model for Surface Chemistry/Optoelectronic Property Relations in Semiconductor Nanocrystals. Journal of the American Chemical Society, 2018, 140, 13292-13300.	13.7	126

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19	Alkyl Phosphonic Acids Deliver CsPbBr₃ Nanocrystals with High Photoluminescence Quantum Yield and Truncated Octahedron Shape. Chemistry of Materials, 2019, 31, 9140-9147.	6.7	125
20	Probing Solventâ€“Ligand Interactions in Colloidal Nanocrystals by the NMR Line Broadening. Chemistry of Materials, 2018, 30, 5485-5492.	6.7	117
21	Ligand Displacement Exposes Binding Site Heterogeneity on CdSe Nanocrystal Surfaces. Chemistry of Materials, 2018, 30, 1178-1186.	6.7	116
22	Epitaxially Connected PbSe Quantum-Dot Films: Controlled Neck Formation and Optoelectronic Properties. ACS Nano, 2014, 8, 11499-11511.	14.6	114
23	On the Nature of Actinideâ€“ and Lanthanideâ€“Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	3.3	112
24	Quantum Chemical Calculations and Experimental Investigations of Molecular Actinide Oxides. Chemical Reviews, 2015, 115, 1725-1759.	47.7	103
25	Continuous-wave infrared optical gain and amplified spontaneous emission at ultralow threshold by colloidal HgTe quantum dots. Nature Materials, 2018, 17, 35-42.	27.5	99
26	Defects in Lead Halide Perovskite Nanocrystals: Analogies and (Many) Differences with the Bulk. ACS Energy Letters, 2019, 4, 2739-2747.	17.4	89
27	A Fock space coupled cluster study on the electronic structure of the UO2, UO2+, U4+, and U5+ species. Journal of Chemical Physics, 2007, 127, 124308.	3.0	88
28	Density of Trap States and Auger-mediated Electron Trapping in CdTe Quantum-Dot Solids. Nano Letters, 2015, 15, 3056-3066.	9.1	84
29	Sb-Doped Metal Halide Nanocrystals: A 0D versus 3D Comparison. ACS Energy Letters, 2021, 6, 2283-2292.	17.4	83
30	Stable Ligand Coordination at the Surface of Colloidal CsPbBr₃ Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 3715-3726.	4.6	77
31	Spectrally Resolved Ultrafast Exciton Transfer in Mixed Perovskite Quantum Wells. Journal of Physical Chemistry Letters, 2019, 10, 419-426.	4.6	74
32	Is Fullerene C₆₀ Large Enough to Host a Multiply Bonded Dimetal?. Journal of the American Chemical Society, 2008, 130, 7459-7465.	13.7	73
33	Ionization Energies for the Actinide Mono- and Dioxides Series, from Th to Cm: Theory versus Experiment. Journal of Physical Chemistry A, 2010, 114, 6007-6015.	2.5	73
34	Benchmark Assessment of Density Functional Methods on Group IIâ€“VI MX (M = Zn, Cd; X = S, Se, Te) Quantum Dots. Journal of Chemical Theory and Computation, 2014, 10, 76-89.	5.3	69
35	Directional Anisotropy of the Vibrational Modes in 2D-Layered Perovskites. ACS Nano, 2020, 14, 4689-4697.	14.6	69
36	Tuning Electronâ€“Phonon Interactions in Nanocrystals through Surface Termination. Nano Letters, 2018, 18, 2233-2242.	9.1	68

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37	Planar pentacoordinate carbons in CBe₅^{4âˆ’} derivatives. Physical Chemistry Chemical Physics, 2015, 17, 4620-4624.	2.8	66
38	Ultra-narrow room-temperature emission from single CsPbBr3 perovskite quantum dots. Nature Communications, 2022, 13, 2587.	12.8	66
39	How accurate are electronic structure methods for actinoid chemistry?. Theoretical Chemistry Accounts, 2011, 129, 657-666.	1.4	65
40	On the performance of the intermediate Hamiltonian Fock-space coupled-cluster method on linear triatomic molecules: The electronic spectra of NpO2+, NpO22+, and PuO22+. Journal of Chemical Physics, 2006, 125, 074301.	3.0	63
41	Compositional Tuning of Carrier Dynamics in Cs₂Na_{1â€“<i>x</i>}Ag_{<i>x</i>}BiCl₆ Double-Perovskite Nanocrystals. ACS Energy Letters, 2020, 5, 1840-1847.	17.4	63
42	Bright Blue Emitting Cu-Doped Cs₂ZnCl₄ Colloidal Nanocrystals. Chemistry of Materials, 2020, 32, 5897-5903.	6.7	63
43	Pro-oxidant Activity of Aluminum: Stabilization of the Aluminum Superoxide Radical Ion. Journal of Physical Chemistry A, 2011, 115, 6717-6723.	2.5	60
44	Fully Inorganic Ruddlesdenâ€“Popper Double Clâ€“I and Triple Clâ€“Brâ€“I Lead Halide Perovskite Nanocrystals. Chemistry of Materials, 2019, 31, 2182-2190.	6.7	60
45	Binding and Packing in Two-Component Colloidal Quantum Dot Ligand Shells: Linear versus Branched Carboxylates. Journal of the American Chemical Society, 2017, 139, 3456-3464.	13.7	58
46	A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe)13 nanocluster. Physical Chemistry Chemical Physics, 2013, 15, 10996.	2.8	57
47	Halide Perovskiteâ€“Lead Chalcohalide Nanocrystal Heterostructures. Journal of the American Chemical Society, 2021, 143, 1435-1446.	13.7	55
48	Infrared Spectroscopy of Discrete Uranyl Anion Complexes. Journal of Physical Chemistry A, 2008, 112, 508-521.	2.5	53
49	Complete vs Restricted Active Space Perturbation Theory Calculation of the Cr₂ Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 1640-1646.	5.3	53
50	Chemically Triggered Formation of Two-Dimensional Epitaxial Quantum Dot Superlattices. ACS Nano, 2016, 10, 6861-6870.	14.6	49
51	Hot-electron transfer in quantum-dot heterojunction films. Nature Communications, 2018, 9, 2310.	12.8	48
52	Role of Surface Reduction in the Formation of Traps in <i>n</i>-Doped IIâ€“VI Semiconductor Nanocrystals: How to Charge without Reducing the Surface. Chemistry of Materials, 2019, 31, 4575-4583.	6.7	48
53	A first-principles study of IIâ€“VI (II = Zn; VI = O, S, Se, Te) semiconductor nanostructures. Journal of Materials Chemistry, 2012, 22, 21453.	6.7	45
54	Alloy CsCd<i>_x</i>Pb_{1â€“<i>x</i>}Br₃ Perovskite Nanocrystals: The Role of Surface Passivation in Preserving Composition and Blue Emission. Chemistry of Materials, 2020, 32, 10641-10652.	6.7	45

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55	Are There Good Alternatives to Lead Halide Perovskite Nanocrystals?. Nano Letters, 2021, 21, 6-9.	9.1	44
56	Electrochemical Control over Photoinduced Electron Transfer and Trapping in CdSe-CdTe Quantum-Dot Solids. ACS Nano, 2014, 8, 7067-7077.	14.6	42
57	Quantum-Confined and Enhanced Optical Absorption of Colloidal PbS Quantum Dots at Wavelengths with Expected Bulk Behavior. Nano Letters, 2017, 17, 1248-1254.	9.1	42
58	The Future of Ligand Engineering in Colloidal Semiconductor Nanocrystals. Accounts of Chemical Research, 2021, 54, 1555-1564.	15.6	42
59	Colloidal Bi-Doped Cs₂Ag_{1â€“<i>x</i>}Na_{<i>x</i>}InCl₆ Nanocrystals: Undercoordinated Surface Cl Ions Limit their Light Emission Efficiency. , 2020, 2, 1442-1449.		41
60	Phonon-Mediated and Weakly Size-Dependent Electron and Hole Cooling in CsPbBr₃ Nanocrystals Revealed by Atomistic Simulations and Ultrafast Spectroscopy. Nano Letters, 2020, 20, 1819-1829.	9.1	41
61	A theoretical study of the ground state and lowest excited states of PuO0/+/+2 and PuO20/+/+2. Physical Chemistry Chemical Physics, 2008, 10, 7278.	2.8	40
62	Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. Journal of Chemical Physics, 2013, 138, 151102.	3.0	38
63	Acidâ€“Base Mediated Ligand Exchange on Near-Infrared Absorbing, Indium-Based IIIâ€“V Colloidal Quantum Dots. Journal of the American Chemical Society, 2021, 143, 4290-4301.	13.7	38
64	Highly Emissive Selfâ€Trapped Excitons in Fully Inorganic Zeroâ€Dimensional Tin Halides. Angewandte Chemie, 2018, 130, 11499-11503.	2.0	37
65	Elucidating the Trends in Reactivity of Azaâ€1,3â€Dipolar Cycloadditions. European Journal of Organic Chemistry, 2019, 2019, 378-386.	2.4	37
66	Ultrathin Orthorhombic PbS Nanosheets. Chemistry of Materials, 2019, 31, 8145-8153.	6.7	37
67	QM/MM study of aqueous solvation of the uranyl fluoride [UO2F42?] complex. Journal of Computational Chemistry, 2004, 25, 386-392.	3.3	35
68	Nanocrystals of Lead Chalcohalides: A Series of Kinetically Trapped Metastable Nanostructures. Journal of the American Chemical Society, 2020, 142, 10198-10211.	13.7	34
69	The Reactivity of CsPbBr₃ Nanocrystals toward Acid/Base Ligands. ACS Nano, 2022, 16, 1444-1455.	14.6	33
70	The importance of spin-orbit coupling and electron correlation in the rationalization of the ground state of the CUO molecule. Journal of Chemical Physics, 2004, 121, 5783-5788.	3.0	32
71	QMflows: A Tool Kit for Interoperable Parallel Workflows in Quantum Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 3191-3197.	5.4	32
72	Infrared Spectra of the WH4(H2)4Complex in Solid Hydrogen. Journal of the American Chemical Society, 2008, 130, 1972-1978.	13.7	31

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73	Cesium Manganese Bromide Nanocrystal Sensitizers for Broadband Vis-to-NIR Downshifting. ACS Energy Letters, 2022, 7, 1850-1858.	17.4	30
74	Experimental and Theoretical Evidence for U(C₆H₆) and Th(C₆H₆) Complexes. Journal of Physical Chemistry A, 2007, 111, 11996-12000.	2.5	28
75	Binding Motifs for Lanthanide Hydrides: A Combined Experimental and Theoretical Study of the MHx(H2)y Species (M = Laâˆ’Gd; x = 1âˆ’4; y = 0âˆ’6). Journal of Physical Chemistry A, 2009, 113, 2446-2455.	2.5	28
76	Ruthenium-Decorated Cobalt Selenide Nanocrystals for Hydrogen Evolution. ACS Applied Nano Materials, 2019, 2, 5695-5703.	5.0	28
77	Modeling Surface Passivation of ZnS Quantum Dots. Journal of Physical Chemistry C, 2012, 116, 2740-2750.	3.1	27
78	Electronic Structure of Ni₂E₂ Complexes (E = S, Se, Te) and a Global Analysis of M₂E₂ Compounds: A Case for Quantized E₂^{<i>n</i>â€“} Oxidation Levels with <i>n</i> = 2, 3, or 4. Journal of the American Chemical Society, 2015, 137, 4993-5011.	13.7	26
79	Noble Gas Matrices May Change the Electronic Structure of Trapped Molecules: The UO₂(Ng)₄ [Ng=Ne, Ar] Case. Chemistry - A European Journal, 2010, 16, 12804-12807.	3.3	25
80	The Surface Chemistry of Colloidal HgSe Nanocrystals, toward Stoichiometric Quantum Dots by Design. Chemistry of Materials, 2018, 30, 7637-7647.	6.7	25
81	Near-Edge Ligand Stripping and Robust Radiative Exciton Recombination in CdSe/CdS Core/Crown Nanoplatelets. Journal of Physical Chemistry Letters, 2020, 11, 3339-3344.	4.6	24
82	The Electronic Structure of the Al₃^{âˆ’} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
83	An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools. Physical Chemistry Chemical Physics, 2012, 14, 8732.	2.8	22
84	Shape, Electronic Structure, and Trap States in Indium Phosphide Quantum Dots. Chemistry of Materials, 2021, 33, 6885-6896.	6.7	22
85	The chemiionization reactions Ce + O and Ce + O₂: Assignment of the observed chemielectron bands. International Journal of Quantum Chemistry, 2009, 109, 2068-2079.	2.0	21
86	Efficient Hot Electron Transfer in Quantum Dot-Sensitized Mesoporous Oxides at Room Temperature. Nano Letters, 2018, 18, 5111-5115.	9.1	21
87	ZnCl₂ Mediated Synthesis of InAs Nanocrystals with Aminoarsine. Journal of the American Chemical Society, 2022, 144, 10515-10523.	13.7	21
88	Quantum Dot Photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer Mechanism Driven by Electronic Coupling. Journal of Physical Chemistry C, 2014, 118, 8712-8721.	3.1	20
89	The effect of TiO₂ surface on the electron injection efficiency in PbS quantum dot solar cells: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 6076-6086.	2.8	20
90	First-Principles Modeling of Core/Shell Quantum Dot Sensitized Solar Cells. Journal of Physical Chemistry C, 2015, 119, 12739-12748.	3.1	20

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91	Dynamic Formation of Metal-Based Traps in Photoexcited Colloidal Quantum Dots and Their Relevance for Photoluminescence. Chemistry of Materials, 2021, 33, 3349-3358.	6.7	20
92	Role of methyl substitution on the spectroscopic properties of porphyrazines. A TDDFT study using pure and hybrid functionals on porphyrazine and its octamethyl derivative. Chemical Physics Letters, 2003, 367, 308-318.	2.6	19
93	Theoretical Study of the Gas-Phase Chemiionization Reactions La + O and La + O₂. Journal of Physical Chemistry A, 2008, 112, 7825-7830.	2.5	19
94	Effect of Ligands and Solvents on the Stability of Electron Charged CdSe Colloidal Quantum Dots. Journal of Physical Chemistry C, 2021, 125, 23968-23975.	3.1	19
95	Limits of Defect Tolerance in Perovskite Nanocrystals: Effect of Local Electrostatic Potential on Trap States. Journal of the American Chemical Society, 2022, 144, 11059-11063.	13.7	19
96	Electronic Structure Engineering Achieved via Organic Ligands in Silicon Nanocrystals. Chemistry of Materials, 2020, 32, 6326-6337.	6.7	17
97	Colloidal Bismuth Chalcohalide Nanocrystals. Angewandte Chemie - International Edition, 2022, 61, .	13.8	17
98	U and P4Reaction Products: A Quantum Chemical and Matrix Isolation Spectroscopic Investigation. Inorganic Chemistry, 2010, 49, 9230-9235.	4.0	16
99	Cs₃Cu₄In₂Cl₁₃ Nanocrystals: A Perovskite-Related Structure with Inorganic Clusters at A Sites. Inorganic Chemistry, 2020, 59, 548-554.	4.0	16
100	Fast Intrinsic Emission Quenching in Cs₄PbBr₆ Nanocrystals. Nano Letters, 2021, 21, 8619-8626.	9.1	16
101	Halide perovskites as disposable epitaxial templates for the phase-selective synthesis of lead sulfochloride nanocrystals. Nature Communications, 2022, 13, .	12.8	16
102	Isolated [SbCl₆]^{3â€“} Octahedra Are the Only Active Emitters in Rb₇Sb₃Cl₁₆ Nanocrystals. ACS Energy Letters, 2021, 6, 3952-3959.	17.4	15
103	Matrix Infrared Spectroscopic and Computational Investigation of Late Lanthanide Metal Hydride Species MH_{<i>x</i>}(H₂)_{<i>y</i>} (M = Tbâ^'Lu, <i>x</i> = 1â^'4, <i>y</i>) Tj ET Qq1 1 0.784314	2.5	14
104	Force Field Parametrization of Colloidal CdSe Nanocrystals Using an Adaptive Rate Monte Carlo Optimization Algorithm. Journal of Chemical Theory and Computation, 2017, 13, 297-308.	5.3	13
105	Ligand Adsorption Energy and the Postpurification Surface Chemistry of Colloidal Metal Chalcogenide Nanocrystals. Chemistry of Materials, 2021, 33, 2796-2803.	6.7	13
106	A QM/MM study on the aqueous solvation of the tetrahydroxouranylate [UO2(OH)4]2â^' complex ion. Journal of Computational Chemistry, 2006, 27, 1156-1162.	3.3	12
107	Electronic Structure and Bonding in Heteronuclear Dimers of V, Cr, Mo, and W: a CASSCF/CASPT2 Study. Inorganic Chemistry, 2011, 50, 9219-9229.	4.0	12
108	Molecules with High Bond Orders and Ultrashort Bond Lengths: CrU, MoU, and WU. Inorganic Chemistry, 2013, 52, 2838-2843.	4.0	12

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109	Electronic spectroscopy and electronic structure of diatomic IrSi. Journal of Chemical Physics, 2013, 138, 154306.	3.0	12
110	An â€œIntermediate Spinâ€•Nickel Hydride Complex Stemming from Delocalized Ni₂(Î¼-H)₂ Bonding. Journal of the American Chemical Society, 2014, 136, 13538-13541.	13.7	12
111	Matrix Infrared Spectroscopy and a Theoretical Investigation of SUO and US2. European Journal of Inorganic Chemistry, 2011, 2011, 4457-4463.	2.0	11
112	Po-Containing Molecules in Fusion and Fission Reactors. Journal of Physical Chemistry Letters, 2019, 10, 2879-2884.	4.6	11
113	A First Theoretical Study on the Origin of the Metal-Mediated Regioselective Opening of 2,3-Epoxy Alcohols. Journal of Organic Chemistry, 2003, 68, 3773-3780.	3.2	9
114	New Investigations of Geometric, Electronic, and Spectroscopic Properties of Tetrapyrrolic Macrocycles by a TDâˆ’DFT Approach. Carbon, Nitrogen, and Chalcogen (O, S, Se) Peripheral Substitution Effects on Ni(II) Porphyrazinato Complexes. Journal of Chemical Theory and Computation, 2007, 3, 838-851.	5.3	9
115	Guidelines for the characterization of metal halide nanocrystals. Trends in Chemistry, 2021, 3, 631-644.	8.5	9
116	Theoretic study of the electronic spectra of neutral and cationic PaO and PaO2. Structural Chemistry, 2013, 24, 917-925.	2.0	8
117	Classical Force-Field Parameters for CsPbBr₃ Perovskite Nanocrystals. Journal of Physical Chemistry C, 2022, 126, 9898-9908.	3.1	8
118	Ion energetics in electron-rich nanoplasmas. New Journal of Physics, 2012, 14, 075017.	2.9	7
119	Theoretical study of the electronic spectra of neutral and cationic NpO and NpO2. Journal of Chemical Physics, 2015, 143, 074305.	3.0	6
120	An Overview of Computational Studies on Colloidal Semiconductor Nanocrystals. Chimia, 2021, 75, 427.	0.6	5
121	Colloidal Bismuth Chalcohalide Nanocrystals. Angewandte Chemie, 2022, 134, .	2.0	5
122	Frontispiece: The Electronic Structure of the Al3âˆ’Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
123	Computational Chemistry to Design Colloidally Stable and Trap-free Perovskite Nanocrystals. , 0, , .		0
124	Size- and Temperature- Dependent Hot Carrier Cooling in CsPbBr3 Nanocrystals. , 0, , .		0
125	The Surface Chemistry of Colloidal II-VI Two-Dimensional Nanoplatelets. , 0, , .		0
126	Phonon-Mediated and Weakly Size-Dependent Electron and Hole Cooling in CsPbBr3 Nanocrystals Revealed by Atomistic Simulations and Ultrafast Spectroscopy. , 0, , .		0