Zoila Barandiaran

List of Publications by Year
in descending order

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107 papers	4,219 citations	109321 35 h-index	128289 60 g-index
118 all docs	118 docs citations	118 times ranked	1951 citing authors

#	Article	IF	Citations
1	Charge transfer from Eu2+ to trivalent lanthanide co-dopants: Systematic behavior across the series. Journal of Chemical Physics, 2021, 154, 064704.	3.0	20
2	Elucidation of the electron transfer mechanism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Eu</mml:mi></mml:mrow><mml:mrow><m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Sm</mml:mi></mml:mrow><mml:mrow><m codoped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml. Physical Review B, 2021, 104, .	3.2	18
3	Insights into the complexity of the excited states of Eu-doped luminescent materials. Inorganic Chemistry Frontiers, 2020, 7, 871-888.	6.0	49
4	Mixed-Valence Lanthanide-Activated Phosphors: Invariance of the Intervalence Charge Transfer (IVCT) Absorption Onset across the Series. Journal of Physical Chemistry C, 2020, 124, 2619-2626.	3.1	15
5	Broadband infrared LEDs based on europium-to-terbium charge transfer luminescence. Nature Communications, 2020, 11, 3647.	12.8	99
6	Fine-Tuning the Cr³⁺ R₁-Line by Controlling Pauli Antisymmetry Strength. Journal of Physical Chemistry Letters, 2019, 10, 3176-3180.	4.6	6
7	Direct Evidence of Intervalence Charge-Transfer States of Eu-Doped Luminescent Materials. Journal of Physical Chemistry Letters, 2019, 10, 1581-1586.	4.6	34
8	X-ray Excitation Triggers Ytterbium Anomalous Emission in CaF₂:Yb but Not in SrF₂:Yb. Journal of Physical Chemistry Letters, 2017, 8, 1175-1178.	4.6	16
9	Energy Level Structure and Multiple 4f¹²5d¹ Emission Bands for Tm²⁺ in Halide Perovskites: Theory and Experiment. Journal of Physical Chemistry C, 2017, 121, 10095-10101.	3.1	24
10	Color Control of Pr³⁺ Luminescence by Electronâ€“Hole Recombination Energy Transfer in CaTiO₃ and CaZrO₃. Journal of Physical Chemistry Letters, 2017, 8, 3095-3100.	4.6	41
11	The Complexity of the CaF₂:Yb System: A Huge, Reversible, X-ray-Induced Valence Reduction. Journal of Physical Chemistry C, 2017, 121, 28435-28442.	3.1	17
12	Evidence That the Anomalous Emission from CaF₂:Yb²⁺ Is Not Described by the Impurity Trapped Exciton Model. Journal of Physical Chemistry Letters, 2017, 8, 3313-3316.	4.6	17
13	New Insights in 4f¹²5d¹ Excited States of Tm²⁺ through Excited State Excitation Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 2730-2734.	4.6	17
14	Ab Initio Calculations on Excited States of Lanthanide Containing Materials. Fundamental Theories of Physics, 2016, 50, 65-89.	0.3	10
15	Red shifts of the yellow emission of YAG:Ce³⁺ due to tetragonal fields induced by cationic substitutions. RSC Advances, 2016, 6, 25741-25743.	3.6	10
16	Metal-to-metal charge transfer between dopant and host ions: Photoconductivity of Yb-doped CaF2 and SrF2 crystals. Journal of Chemical Physics, 2015, 143, 144702.	3.0	15
17	Structural relaxation effects on the lowest $$4f{-}5d$$ 4 f - 5 d transition of $$hbox {Ce}^{3+}$$ Ce 3 + in garnets. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	12
18	Configuration coordinate energy level diagrams of intervalence and metal-to-metal charge transfer states of dopant pairs in solids. Physical Chemistry Chemical Physics, 2015, 17, 19874-19884.	2.8	64

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19	Anomalous Red and Infrared Luminescence of Ce³⁺ Ions in SrS:Ce Sintered Ceramics. Journal of Physical Chemistry C, 2015, 119, 27649-27656.	3.1	14
20	Intervalence charge transfer luminescence: Interplay between anomalous and 5d â^' 4f emissions in Yb-doped fluorite-type crystals. Journal of Chemical Physics, 2014, 141, 234704.	3.0	56
21	Intervalence charge transfer luminescence: The anomalous luminescence of cerium-doped Cs2LiLuCl6 elpasolite. Journal of Chemical Physics, 2014, 141, 214706.	3.0	32
22	Ab initio theoretical study of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0291.gif" overflow="scroll"><mml:mn>4</mml:mn><mml:msup><mml:mrow><mml:mi mathvariant="normal">f</mml:mi></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow></mml:msup></mml:math> and 4f75d manifolds of Tb3+-doped BaF2 cubic sites. Journal of Luminescence, 2014, 145, 808-817.	3.1	20
23	Ab initio Theoretical Study on the 4f² and 4f5d Electronic Manifolds of Cubic Defects in CaF₂:Pr³⁺. Journal of Physical Chemistry A, 2014, 118, 358-368.	2.5	28
24	Large splittings of the 4f shell of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2014, 16, 3830.	2.8	35
25	Blue absorption and red emission of Bi²⁺ in solids: strongly spinâ€“orbit coupled 6p levels in low symmetry fields. Physical Chemistry Chemical Physics, 2014, 16, 17305-17314.	2.8	13
26	Structure and Hindered Vibration of Bi²⁺ in the Red-Orange Phosphor SrB₄O₇:Bi. Journal of Physical Chemistry C, 2014, 118, 17932-17939.	3.1	15
27	Is Bi²⁺ Responsible for the Red-Orange Emission of Bismuth-Doped SrB₄O₇?. Journal of Physical Chemistry C, 2014, 118, 9696-9705.	3.1	38
28	Host effects on the optically active 4f and 5d levels of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2013, 15, 19221.	2.8	36
29	Radial correlation effects on interconfigurational excitations at the end of the lanthanide series: A restricted active space second order perturbation study of Yb2+ and SrCl2:Yb2+. Journal of Chemical Physics, 2013, 138, 074102.	3.0	25
30	4f and 5d Levels of Ce3+ in D2 8-fold oxygen coordination. Optical Materials, 2013, 35, 1932-1940.	3.6	42
31	Effective Hamiltonian parameters forab initioenergy-level calculations of SrCl₂:Yb²⁺and CsCaBr₃:Yb²⁺. Journal of Physics Condensed Matter, 2013, 25, 415504.	1.8	10
32	Antisite defects in Ce-doped YAG (Y3Al5O12): first-principles study on structures and 4fâ€“5d transitions. Journal of Materials Chemistry, 2012, 22, 19888.	6.7	38
33	Ab initio theoretical study of luminescence properties of Pr3+-doped Lu2O3. Theoretical Chemistry Accounts, 2011, 129, 545-554.	1.4	17
34	Energy level shifts in two-step spinâ€“orbit coupling ab initio calculations. Chemical Physics Letters, 2010, 498, 226-228.	2.6	8
35	Yb 2 + -doped SrCl2: Electronic structure of impurity states and impurity-trapped excitons. Journal of Chemical Physics, 2010, 133, 114509.	3.0	42
36	Electronic spectra of Yb2+-doped SrCl2. Journal of Chemical Physics, 2010, 133, 114506.	3.0	26

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37	Energy Shift of the 4f¹³6s¹Excited States of Yb²⁺from Gas Phase to the CsCaBr₃Solid. Spectroscopy Letters, 2010, 43, 393-399.	1.0	9
38	Structural effects and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi><mml:mtext>â^'</mml:mtext><mml:mn>5</mml:mn><mml:mi shifts induced by La codoping in Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	54
39	Improved Embedding Ab Initio Model Potentials for Embedded Cluster Calculations. Journal of Physical Chemistry A, 2009, 113, 12454-12460.	2.5	24
40	Spin-forbidden and spin-enabled 4f14â†'4f135d1 transitions of Yb2+-doped CsCaBr3. Journal of Chemical Physics, 2009, 131, 024505.	3.0	22
41	Energy Gaps in the 4f¹³5d¹ Manifold and Multiple Spontaneous Emissions in Yb²⁺-Doped CsCaBr₃. Journal of Physical Chemistry A, 2009, 113, 12591-12598.	2.5	30
42	Ab initio calculations on the local structure and the 4fâ€“5d absorption and emission spectra of -doped YAG. Journal of Luminescence, 2008, 128, 1248-1254.	3.1	93
43	Embedding Fragment ab Initio Model Potentials in CASSCF/CASPT2 Calculations of Doped Solids: Implementation and Applications. Journal of Chemical Theory and Computation, 2008, 4, 586-594.	5.3	50
44	Geometry and electronic structure of impurity-trapped excitons in Cs2GeF6:U4+ crystals. The 5f17s1 manifold. Journal of Chemical Physics, 2007, 126, 194712.	3.0	21
45	Detailed interpretation of the 5f-6d absorption spectrum of U3+ in Cs2NaYCl6 and high pressure effects based on an ab initio simulation. Journal of Chemical Physics, 2007, 127, 144712.	3.0	10
46	Relation between high-pressure spectroscopy and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>f</mml:mi><mml:mrow><mml:mi>n</mml:mi><mml:mo>â^'</mml:mo><mml:mn> geometry: A comparison between theoretical and experimental results in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant=. Physical Review B, 2007, 76, .	3.2	20
47	The 5f3 manifold of the free-ion U3+: Ab initio calculations. Chemical Physics Letters, 2007, 434, 1-5.	2.6	13
48	The luminescence spectrum of in 2GeF6 crystalsâ€"A quantum chemical study. Journal of Luminescence, 2007, 126, 779-783.	3.1	18
49	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. Theoretical Chemistry Accounts, 2007, 118, 541-547.	1.4	10
50	Large anomalies due to insufficiency of Madelung embedding inab initiocalculations of4fâ^'5dand4fâ^'6sexcitations of lanthanides in ionic crystals: TheBaF2:Ce3+crystal. Physical Review B, 2006, 74, .	3.2	28
51	On the Bond Length Change upon 4f 1 â†' 5d 1 Excitations in Eightfold Coordination: CaF2:Ce3+ Cubic Defects. Theoretical Chemistry Accounts, 2006, 116, 505-508.	1.4	15
52	Theoretical study of the effects of F to Cl chemical substitution on the electronic structure and the luminescence properties of Cs2GeF6:Os4+ and Cs2ZrCl6:Os4+ materials. Journal of Chemical Physics, 2006, 124, 124315.	3.0	8
53	The 5f2â†'5f16d1 absorption spectrum of Cs2GeF6:U4+ crystals: A quantum chemical and experimental study. Journal of Chemical Physics, 2006, 125, 074511.	3.0	22
54	Bond lengths of and states of hexahalides. Journal of Solid State Chemistry, 2005, 178, 464-469.	2.9	40

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55	Quantum chemical study of 4fâ†'5d excitations of trivalent lanthanide ions doped in the cubic elpasolite Cs2NaYCl6. Ce3+ to Tb3+. Journal of Chemical Physics, 2005, 123, 244703.	3.0	30
56	5fâ†'5f transitions of U4+ ions in high-field, octahedral fluoride coordination: The Cs2GeF6:U4+ crystal. Journal of Chemical Physics, 2005, 123, 204502.	3.0	19
57	Prediction of pressure-induced redshift of f1â†'d(t2g)1 excitations in Cs2NaYCl6:Ce3+ and its connection with bond-length shortening. Journal of Chemical Physics, 2005, 122, 234507.	3.0	19
58	Parallel, linear-scaling building-block and embedding method based on localized orbitals and orbital-specific basis sets. Journal of Chemical Physics, 2004, 121, 6698-6709.	3.0	27
59	Relativistic Ab-Initio Model Potential Calculations for Molecules and Embedded Clusters. Theoretical and Computational Chemistry, 2004, , 417-475.	0.4	12
60	Absorption and Emission Spectra of Ce3+in Elpasolite Lattices. Journal of the American Chemical Society, 2003, 125, 13225-13233.	13.7	95
61	Transferability of core potentials to f and d states of lanthanide and actinide ions. Molecular Physics, 2003, 101, 73-80.	1.7	75
62	Quantum chemical study of the lanthanide bond length contraction on Ln3+-doped Cs2NaYCl6 crystals (Ln=Ce to Lu). Journal of Chemical Physics, 2003, 119, 6143-6149.	3.0	16
63	Quantum chemical analysis of the bond lengths in fn and fnâˆ'1d1 states of Ce3+, Pr3+, Pa4+, and U4+ defects in chloride hosts. Journal of Chemical Physics, 2003, 119, 3785-3790.	3.0	52
64	Ab initio theoretical studies on U3+ and on the structure and spectroscopy of U3+ substitutional defects in Cs2NaYCl6, 5fâ€Š26d1 manifold. Journal of Chemical Physics, 2003, 118, 5335-5346.	3.0	43
65	High pressure effects on the structure and spectroscopy of V3+ substitutional defects in Cs2NaYCl6. Anab initioembedded cluster study. Journal of Chemical Physics, 2003, 118, 1921-1928.	3.0	15
66	Structure and spectroscopy of U[sup 4+] defects in Cs[sub 2]ZrCl[sub 6]: Ab initio theoretical studies on the 5fâ€Š[sup 2] and 5fâ€Š[sup 1]6d[sup 1] manifolds. Journal of Chemical Physics, 2003, 118, 7439.	3.0	46
67	On the nature of the ground state of Cr(V) defects in YVO4: An ab initio model potential embedded-cluster study. International Journal of Quantum Chemistry, 2002, 90, 751-758.	2.0	2
68	The ab initio model potential method: Lanthanide and actinide elements. Journal of Chemical Physics, 2001, 114, 118.	3.0	75
69	Ab initio model potential embedded-cluster calculation of the geometric structure of Tl+ monomer and dimer centers in KCl. Computational and Theoretical Chemistry, 2001, 537, 151-161.	1.5	2
70	Structure and spectroscopy of Pa4+ defects in Cs2ZrCl6. An ab initio theoretical study. Journal of Chemical Physics, 2001, 115, 5554-5560.	3.0	32
71	Alternative configuration interaction expansions for transition metal ions with intermediate oxidation states in crystals: The structure and absorption spectrum of Cs2GeF6:Mn4+. Journal of Chemical Physics, 2001, 115, 7061-7065.	3.0	15
72	Structure and spectroscopy of Cr3+ defects in KMgF3, KZnF3, and CsCaF3 crystals. An ab initio model potential embedded cluster study. International Journal of Quantum Chemistry, 2000, 77, 961-972.	2.0	14

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73	Ab initio model potential embedded cluster calculation of the absorption spectrum of Cs2GeF6:Mn4+. Large discrepancies between theory and experiment. International Journal of Quantum Chemistry, 2000, 80, 623-635.	2.0	16
74	The Ab Initio Model Potential Method: A Common Strategy for Effective Core Potential and Embedded Cluster Calculations. Computational Chemistry - Reviews of Current Trends, 1999, , 55-152.	0.4	89
75	Ab initio model potential embedded cluster study of the structure and spectroscopy of V3+-doped elpasolites K2NaScF6, Cs2NaYCl6 and Cs2NaYBr6. Computational and Theoretical Chemistry, 1998, 451, 135-142.	1.5	6
76	A new interpretation of the bonding and spectroscopy of the tetraoxoferrate(VI) FeO42â^' ion. Journal of Chemical Physics, 1998, 109, 6396-6405.	3.0	14
77	Ab initiomodel potential embedded-cluster study of the ground and lowest excited states of Cr3+ defects in the elpasolites Cs2NaYCl6 and Cs2NaYBr6. Journal of Chemical Physics, 1998, 108, 2005-2014.	3.0	38
78	Multiple-excited-state absorption ofV2+in low-field crystals: Anab initiomodel-potential embedded-cluster study. Physical Review B, 1998, 57, 11974-11979.	3.2	10
79	Applications of the group-function theory to the field of materials science. International Journal of Quantum Chemistry, 1996, 60, 617-634.	2.0	41
80	Ab initio model potential calculations on the electronic spectrum of Ni2+â€doped MgO including correlation, spinâ€“orbit and embedding effects. Journal of Chemical Physics, 1996, 105, 5321-5330.	3.0	135
81	Ab initiomodel-potential embedded-cluster study of Jahn-Teller parameters and electronic transition energies ofCr2+in oxide and fluoride octahedral coordination. Physical Review B, 1996, 53, 1138-1145.	3.2	11
82	Excitedâ€state absorption spectra of V2+â€doped fluoroperovskites. An ab initio model potential embeddedâ€cluster study. Journal of Chemical Physics, 1996, 105, 50-61.	3.0	17
83	Ab initio model potential embeddedâ€cluster study of V2+â€doped fluoroperovskites: Effects of different hosts on the local distortion and electronic structure of 4T2gâ€“4A2g laser levels. Journal of Chemical Physics, 1995, 103, 2117-2125.	3.0	34
84	Ab initio model potential study of the optical absorption spectrum of Mn2+â€doped CaF2. Journal of Chemical Physics, 1995, 103, 4841-4846.	3.0	12
85	Quasirelativistic ab initio model potential calculations on the group IV hydrides (XH2, XH4;) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	3.0	56
86	Bonding between CO and the MgO(001) surface: A modified picture. Journal of Chemical Physics, 1994, 100, 2010-2018.	3.0	186
87	Ab initio model potential study of pressure effects on K2NaGaF6:Cr3+. Journal of Chemical Physics, 1993, 98, 4041-4046.	3.0	40
88	Ab initio model potential study of environmental effects on the Jahnâ€“Teller parameters of Cu2+ and Ag2+ impurities in MgO, CaO, and SrO hosts. Journal of Chemical Physics, 1993, 98, 9715-9724.	3.0	83
89	The abinitio model potential method. Cowanâ€“Griffin relativistic core potentials and valence basis sets from Li (Zâ€,=â€,3) to La (Zâ€,=â€,57). Canadian Journal of Chemistry, 1992, 70, 409-415.	1.1	214
90	Self-consistent embedded clusters: Building block equations for localized orthogonal orbitals. Journal of Mathematical Chemistry, 1992, 10, 41-56.	1.5	29

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91	Atomic valence correlation energies from ab initio model potential calculations. Chemical Physics Letters, 1992, 192, 217-220.	2.6	11
92	Ab initio model potential study of the equilibrium geometry of alkaline earth dihalides: MX2 (M=Mg,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.0	100
93	Ab initio model potential study of local distortions around Cr+ and Cr3+ defects in fluorite. Journal of Chemical Physics, 1991, 94, 8158-8164.	3.0	48
94	The ab initio model potential method. Second series transition metal elements. Journal of Chemical Physics, 1990, 93, 5843-5850.	3.0	86
95	The ab initio model potential method. First series transition metal elements. Journal of Chemical Physics, 1989, 91, 7011-7017.	3.0	80
96	The ab initio model potential representation of the crystalline environment. Theoretical study of the local distortion on NaCl:Cu+. Journal of Chemical Physics, 1988, 89, 5739-5746.	3.0	373
97	The ab initio model potential method. Main group elements. Journal of Chemical Physics, 1987, 86, 2132-2145.	3.0	245
98	Towards HF SCF value of electron affinity of SF6. Journal of Chemical Physics, 1987, 86, 1637-1638.	3.0	32
99	Ab initio SCF studies of the molecular structure of XeF6, IF 6 ? , and TeF 6 2? in non-octahedral geometries. Theoretica Chimica Acta, 1987, 71, 237-245.	0.8	24
100	Extended model potential calculations on I2 and HI molecules. Journal of Chemical Physics, 1986, 84, 1941-1942.	3.0	7
101	Core-projection effects in near ab initio valence calculations of the electronic ground state of the octahedral CrF4â^'6. Journal of Solid State Chemistry, 1986, 61, 269-276.	2.9	15
102	Model potentials suitable for calculations with slater-type basis for Sc through Zn. Journal of Solid State Chemistry, 1986, 61, 277-292.	2.9	5
103	Structure and properties of transition-metal compounds. A systematic study of basis set effects inab initioSCF calculations. International Journal of Quantum Chemistry, 1986, 29, 1047-1058.	2.0	17
104	A systematic study of basis set effects inabinitioSCF calculations: Wellâ€tempered Gaussianâ€type function basis set calculations on transition metal halides. Journal of Chemical Physics, 1986, 84, 6315-6327.	3.0	27
105	Ab initio calculations on transition metal compounds using small minimal GTO basis sets. Chemical Physics Letters, 1985, 117, 151-153.	2.6	21
106	New developments in the model potential method: ScO molecule. Journal of Chemical Physics, 1985, 83, 4565-4572.	3.0	32
107	On the importance of an accurate representation of the Ewald potential throughout the cluster volume in the calculation of the cluster-lattice interaction. Journal of Solid State Chemistry, 1984, 55, 236-238.	2.9	7