Zoila Barandiaran

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1036901/publications.pdf

Version: 2024-02-01

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	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
2	The ab initio model potential method. Main group elements. Journal of Chemical Physics, 1987, 86, 2132-2145.	3.0	245
3	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
4	Bonding between CO and the MgO(001) surface: A modified picture. Journal of Chemical Physics, 1994, 100, 2010-2018.	3.0	186
5	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
6	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
7	Broadband infrared LEDs based on europium-to-terbium charge transfer luminescence. Nature Communications, 2020, 11, 3647.	12.8	99
8	Absorption and Emission Spectra of Ce3+in Elpasolite Lattices. Journal of the American Chemical Society, 2003, 125, 13225-13233.	13.7	95
9	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
10	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
11	The ab initio model potential method. Second series transition metal elements. Journal of Chemical Physics, 1990, 93, 5843-5850.	3.0	86
12	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
13	The ab initio model potential method. First series transition metal elements. Journal of Chemical Physics, 1989, 91, 7011-7017.	3.0	80
14	The ab initio model potential method: Lanthanide and actinide elements. Journal of Chemical Physics, 2001, 114, 118.	3.0	75
15	Transferability of core potentials to f and d states of lanthanide and actinide ions. Molecular Physics, 2003, 101, 73-80.	1.7	75
16	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
17	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
18	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

#	Article	IF	Citations
19	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:mn shifts induced by La codoping in Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	54
20	Quantum chemical analysis of the bond lengths in fn and fnâ^'1d1 states of Ce3+, Pr3+, Pa4+, and U4+ defects in chloride hosts. Journal of Chemical Physics, 2003, 119, 3785-3790.	3.0	52
21	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
22	Insights into the complexity of the excited states of Eu-doped luminescent materials. Inorganic Chemistry Frontiers, 2020, 7, 871-888.	6.0	49
23	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
24	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
25	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
26	Yb 2 + -doped SrCl2: Electronic structure of impurity states and impurity-trapped excitons. Journal of Chemical Physics, 2010, 133, 114509.	3.0	42
27	4f and 5d Levels of Ce3+ in D2 8-fold oxygen coordination. Optical Materials, 2013, 35, 1932-1940.	3.6	42
28	Applications of the group-function theory to the field of materials science. International Journal of Quantum Chemistry, 1996, 60, 617-634.	2.0	41
29	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
30	Ab initio model potential study of pressure effects on K2NaGaF6:Cr3+. Journal of Chemical Physics, 1993, 98, 4041-4046.	3.0	40
31	Bond lengths of and states of hexahalides. Journal of Solid State Chemistry, 2005, 178, 464-469.	2.9	40
32	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
33	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
34	Is Bi²⁺ Responsible for the Red-Orange Emission of Bismuth-Doped SrB₄O₇?. Journal of Physical Chemistry C, 2014, 118, 9696-9705.	3.1	38
35	Host effects on the optically active 4f and 5d levels of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2013, 15, 19221.	2.8	36
36	Large splittings of the 4f shell of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2014, 16, 3830.	2.8	35

#	Article	IF	Citations
37	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
38	Direct Evidence of Intervalence Charge-Transfer States of Eu-Doped Luminescent Materials. Journal of Physical Chemistry Letters, 2019, 10, 1581-1586.	4.6	34
39	New developments in the model potential method: ScO molecule. Journal of Chemical Physics, 1985, 83, 4565-4572.	3.0	32
40	Towards HF SCF value of electron affinity of SF6. Journal of Chemical Physics, 1987, 86, 1637-1638.	3.0	32
41	Structure and spectroscopy of Pa4+ defects in Cs2ZrCl6. An ab initio theoretical study. Journal of Chemical Physics, 2001, 115, 5554-5560.	3.0	32
42	Intervalence charge transfer luminescence: The anomalous luminescence of cerium-doped Cs2LiLuCl6 elpasolite. Journal of Chemical Physics, 2014, 141, 214706.	3.0	32
43	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
44	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
45	Self-consistent embedded clusters: Building block equations for localized orthogonal orbitals. Journal of Mathematical Chemistry, 1992, 10, 41-56.	1.5	29
46	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
47	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
48	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
49	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
50	Electronic spectra of Yb2+-doped SrCl2. Journal of Chemical Physics, 2010, 133, 114506.	3.0	26
51	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
52	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
53	Improved Embedding Ab Initio Model Potentials for Embedded Cluster Calculations. Journal of Physical Chemistry A, 2009, 113, 12454-12460.	2.5	24
54	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

#	Article	IF	Citations
55	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
56	Spin-forbidden and spin-enabled 4f14â†'4f135d1 transitions of Yb2+-doped CsCaBr3. Journal of Chemical Physics, 2009, 131, 024505.	3.0	22
57	Ab initio calculations on transition metal compounds using small minimal GTO basis sets. Chemical Physics Letters, 1985, 117, 151-153.	2.6	21
58	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
59	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:m> 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	3.2	20
60	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
61	Charge transfer from Eu2+ to trivalent lanthanide co-dopants: Systematic behavior across the series. Journal of Chemical Physics, 2021, 154, 064704.	3.0	20
62	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
63	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
64	The luminescence spectrum of in 2GeF6 crystalsâ€"A quantum chemical study. Journal of Luminescence, 2007, 126, 779-783.	3.1	18
65	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
66	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
67	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
68	Ab initio theoretical study of luminescence properties of Pr3+-doped Lu2O3. Theoretical Chemistry Accounts, 2011, 129, 545-554.	1.4	17
69	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
70	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
71	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
72	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

#	Article	IF	Citations
73	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
74	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
75	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
76	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
77	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
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	The 5f3 manifold of the free-ion U3+: Ab initio calculations. Chemical Physics Letters, 2007, 434, 1-5.	2.6	13
86	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
87	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
88	Relativistic Ab-Initio Model Potential Calculations for Molecules and Embedded Clusters. Theoretical and Computational Chemistry, 2004, , 417-475.	0.4	12
89	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
90	Atomic valence correlation energies from ab initio model potential calculations. Chemical Physics Letters, 1992, 192, 217-220.	2.6	11

#	Article	IF	Citations
91	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
92	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
93	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
94	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. Theoretical Chemistry Accounts, 2007, 118, 541-547.	1.4	10
95	Effective Hamiltonian parameters forab initioenergy-level calculations of SrCl₂:Yb²⁺and CsCaBr₃:Yb²⁺. Journal of Physics Condensed Matter, 2013, 25, 415504.	1.8	10
96	Ab Initio Calculations on Excited States of Lanthanide Containing Materials. Fundamental Theories of Physics, 2016, 50, 65-89.	0.3	10
97	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
98	Energy Shift of the 4f¹³6s¹Excited States of Yb²⁺from Gas Phase to the CsCaBr₃Solid. Spectroscopy Letters, 2010, 43, 393-399.	1.0	9
99	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
100	Energy level shifts in two-step spinâ€“orbit coupling ab initio calculations. Chemical Physics Letters, 2010, 498, 226-228.	2.6	8
101	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
102	Extended model potential calculations on I2 and HI molecules. Journal of Chemical Physics, 1986, 84, 1941-1942.	3.0	7
103	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
104	Fine-Tuning the Cr³⁺ R₁-Line by Controlling Pauli Antisymmetry Strength. Journal of Physical Chemistry Letters, 2019, 10, 3176-3180.	4.6	6
105	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
106	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
107	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