Luis Seijo

List of Publications by Year
in descending order

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141 papers	7,279 citations	76326 40 h-index	60623 81 g-index
156 all docs	156 docs citations	156 times ranked	4548 citing authors

#	Article	IF	Citations
1	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	3.0	1,689
2	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
3	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
4	The ab initio model potential method. Main group elements. Journal of Chemical Physics, 1987, 86, 2132-2145.	3.0	245
5	Resolving the ambiguity in the relation between Stokes shift and Huangâ€“Rhys parameter. Physical Chemistry Chemical Physics, 2015, 17, 16959-16969.	2.8	226
6	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
7	Bonding between CO and the MgO(001) surface: A modified picture. Journal of Chemical Physics, 1994, 100, 2010-2018.	3.0	186
8	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
9	Relativisticab initiomodel potential calculations including spinâ€“orbit effects through the Woodâ€“Boring Hamiltonian. Journal of Chemical Physics, 1995, 102, 8078-8088.	3.0	101
10	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
11	Broadband infrared LEDs based on europium-to-terbium charge transfer luminescence. Nature Communications, 2020, 11, 3647.	12.8	99
12	Absorption and Emission Spectra of Ce3+in Elpasolite Lattices. Journal of the American Chemical Society, 2003, 125, 13225-13233.	13.7	95
13	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
14	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
15	The ab initio model potential method. Second series transition metal elements. Journal of Chemical Physics, 1990, 93, 5843-5850.	3.0	86
16	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
17	The ab initio model potential method. First series transition metal elements. Journal of Chemical Physics, 1989, 91, 7011-7017.	3.0	80
18	The ab initio model potential method: Lanthanide and actinide elements. Journal of Chemical Physics, 2001, 114, 118.	3.0	75

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19	Transferability of core potentials to f and d states of lanthanide and actinide ions. Molecular Physics, 2003, 101, 73-80.	1.7	75
20	Structural, electronic, and spectroscopic effects of Ga codoping on Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	70
21	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
22	Ab initio model potential embedded cluster calculations including lattice relaxation and polarization: Local distortions on Mn2+â€doped CaF2. Journal of Chemical Physics, 1995, 102, 5368-5376.	3.0	63
23	Geometry and electronic structure ofM-DNA (M=Zn2+,Co2+, andFe2+). Physical Review B, 2006, 73, .	3.2	60
24	Quasirelativistic ab initio model potential calculations on the group IV hydrides (XH2, XH4;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 542 T	3.0	56
25	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
26	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:m shifts induced by La codoping in Ce-doped yttrium aluminum garnet: First-principles study. Physical Review B, 2010, 82, .	3.2	54
27	The ab initio model potential method: Third-series transition metal elements. Journal of Chemical Physics, 1999, 110, 784-796.	3.0	53
28	Electronic properties and 4f â†' 5d transitions in Ce-doped Lu2SiO5: a theoretical investigation. Journal of Materials Chemistry, 2012, 22, 13723.	6.7	53
29	Broadband anti-Stokes white emission of Sr₂CeO₄ nanocrystals induced by laser irradiation. Physical Chemistry Chemical Physics, 2016, 18, 27921-27927.	2.8	53
30	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
31	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
32	Spin-free relativistic no-pair ab initio core model potentials and valence basis sets for the transition metal elements Sc to Hg. Part I. Journal of Chemical Physics, 1999, 110, 3678-3686.	3.0	49
33	Insights into the complexity of the excited states of Eu-doped luminescent materials. Inorganic Chemistry Frontiers, 2020, 7, 871-888.	6.0	49
34	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
35	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
36	Ce and La Single- and Double-Substitutional Defects in Yttrium Aluminum Garnet: First-Principles Study. Journal of Physical Chemistry A, 2011, 115, 815-823.	2.5	46

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37	Atomistic and electronic structure of antisite defects in yttrium aluminum garnet: Density-functional study. Physical Review B, 2009, 80, .	3.2	45
38	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
39	Yb 2 + -doped SrCl2: Electronic structure of impurity states and impurity-trapped excitons. Journal of Chemical Physics, 2010, 133, 114509.	3.0	42
40	4f and 5d Levels of Ce3+ in D2 8-fold oxygen coordination. Optical Materials, 2013, 35, 1932-1940.	3.6	42
41	Applications of the group-function theory to the field of materials science. International Journal of Quantum Chemistry, 1996, 60, 617-634.	2.0	41
42	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
43	Ab initio model potential study of pressure effects on K2NaGaF6:Cr3+. Journal of Chemical Physics, 1993, 98, 4041-4046.	3.0	40
44	Bond lengths of and states of hexahalides. Journal of Solid State Chemistry, 2005, 178, 464-469.	2.9	40
45	Firstâ€principles study of the structure and the electronic structure of yttrium aluminum garnet Y₃Al₅O₁₂. International Journal of Quantum Chemistry, 2009, 109, 1991-1998.	2.0	40
46	Spin-free relativistic no-pair ab initio core model potentials and valence basis sets for the transition metal elements Sc to Hg. II. Journal of Chemical Physics, 1999, 111, 10436-10443.	3.0	39
47	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
48	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
49	Is Bi²⁺ Responsible for the Red-Orange Emission of Bismuth-Doped SrB₄O₇?. Journal of Physical Chemistry C, 2014, 118, 9696-9705.	3.1	38
50	Theoretical calculation of the pure electronic spectrum ofMnF64â^'invacuoand inRbMnF3. Physical Review B, 1986, 34, 1200-1214.	3.2	37
51	Host effects on the optically active 4f and 5d levels of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2013, 15, 19221.	2.8	36
52	Large splittings of the 4f shell of Ce3+ in garnets. Physical Chemistry Chemical Physics, 2014, 16, 3830.	2.8	35
53	Direct Evidence of Intervalence Charge-Transfer States of Eu-Doped Luminescent Materials. Journal of Physical Chemistry Letters, 2019, 10, 1581-1586.	4.6	34
54	New developments in the model potential method: ScO molecule. Journal of Chemical Physics, 1985, 83, 4565-4572.	3.0	32

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55	Towards HF SCF value of electron affinity of SF6. Journal of Chemical Physics, 1987, 86, 1637-1638.	3.0	32
56	Structure and spectroscopy of Pa4+ defects in Cs2ZrCl6. An ab initio theoretical study. Journal of Chemical Physics, 2001, 115, 5554-5560.	3.0	32
57	Intervalence charge transfer luminescence: The anomalous luminescence of cerium-doped Cs2LiLuCl6 elpasolite. Journal of Chemical Physics, 2014, 141, 214706.	3.0	32
58	Third-order Douglasâ€“Kroll ab initio model potential for actinide elements. Journal of Chemical Physics, 2002, 117, 3597-3604.	3.0	31
59	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
60	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
61	Self-consistent embedded clusters: Building block equations for localized orthogonal orbitals. Journal of Mathematical Chemistry, 1992, 10, 41-56.	1.5	29
62	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
63	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
64	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
65	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
66	Electronic spectra of Yb2+-doped SrCl2. Journal of Chemical Physics, 2010, 133, 114506.	3.0	26
67	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
68	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
69	Improved Embedding Ab Initio Model Potentials for Embedded Cluster Calculations. Journal of Physical Chemistry A, 2009, 113, 12454-12460.	2.5	24
70	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
71	The ab initio model potential method with the spin-free relativistic scheme by eliminating small components Hamiltonian. Journal of Chemical Physics, 2001, 114, 6000-6006.	3.0	23
72	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

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73	Spin-forbidden and spin-enabled 4f14â†'4f135d1 transitions of Yb2+-doped CsCaBr3. Journal of Chemical Physics, 2009, 131, 024505.	3.0	22
74	First-Principles Study on Structural Properties and 4f â†' 5d Transitions of Locally Charge-Compensated Ce³⁺ in CaF₂. Journal of Physical Chemistry C, 2012, 116, 18419-18426.	3.1	22
75	Ab initio calculations on transition metal compounds using small minimal GTO basis sets. Chemical Physics Letters, 1985, 117, 151-153.	2.6	21
76	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
77	A third-order Douglasâ€“Kroll ab initio model potential for the lanthanides. Chemical Physics Letters, 2002, 361, 334-340.	2.6	20
78	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>	3.2	20
79	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
80	Charge transfer from Eu2+ to trivalent lanthanide co-dopants: Systematic behavior across the series. Journal of Chemical Physics, 2021, 154, 064704.	3.0	20
81	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
82	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
83	The luminescence spectrum of in 2GeF6 crystalsâ€"A quantum chemical study. Journal of Luminescence, 2007, 126, 779-783.	3.1	18
84	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:mi. Physical Review B, 2021, 104, .	3.2	18
85	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
86	The ab initio model potential method. Relativistic Wood-Boring valence spin-orbit potentials and spin-orbit-corrected basis sets from B(Z = 5) to Ba(Z = 56). Computational and Theoretical Chemistry, 1998, 426, 59-74.	1.5	17
87	Ab initio theoretical study of luminescence properties of Pr3+-doped Lu2O3. Theoretical Chemistry Accounts, 2011, 129, 545-554.	1.4	17
88	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
89	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
90	The maximum overlap method: A general and efficient scheme for reducing basis sets. Application to the generation of approximate AO's for the 3d transition metal atoms and ions. Journal of Solid State Chemistry, 1986, 63, 391-400.	2.9	16

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91	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
92	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
93	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
94	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
95	Theoretical and Experimental Study of Tri- and Tetrahalodiorganostannate(IV) Salts. Solvent Dependence in the Reaction of Dimethyltin Dibromide with Tetraethylammonium Bromide. Organometallics, 2001, 20, 654-662.	2.3	15
96	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
97	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
98	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
99	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
100	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
101	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
102	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
103	Ab initio spin-free-state-shifted spin-orbit configuration interaction calculations on singly ionized iridium. Journal of Chemical Physics, 1998, 108, 7980-7987.	3.0	14
104	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
105	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
106	Quintet-triplet electronic transitions and nephelauxetic effects in CrF4â^'6. Results of an SCF MO calculation. Journal of Solid State Chemistry, 1982, 42, 28-40.	2.9	13
107	The 5f3 manifold of the free-ion U3+: Ab initio calculations. Chemical Physics Letters, 2007, 434, 1-5.	2.6	13
108	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

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109	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
110	Relativistic Ab-Initio Model Potential Calculations for Molecules and Embedded Clusters. Theoretical and Computational Chemistry, 2004, , 417-475.	0.4	12
111	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
112	Atomic valence correlation energies from ab initio model potential calculations. Chemical Physics Letters, 1992, 192, 217-220.	2.6	11
113	Relativistic Wood-Boring ab initio model potential calculations on the platinum atom. Chemical Physics Letters, 1995, 236, 510-515.	2.6	11
114	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
115	Wood-Boring ab initio model potential relativistic treatment of Ce and CeO. Chemical Physics Letters, 1999, 299, 613-622.	2.6	11
116	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>5</mml:mn><mml:mi>f</mml:mi><mml:mtext>â^'</mml:mtext><mml:mn>6</mml:mn><mml:r hybridization of trivalent uranium in crystals of hexagonal symmetry: Effects on electronic energy levels and transition intensities. Physical Review B, 2009, 80, .	3.2	11
117	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
118	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
119	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. Theoretical Chemistry Accounts, 2007, 118, 541-547.	1.4	10
120	Effective Hamiltonian parameters forab initioenergy-level calculations of SrCl₂:Yb²⁺and CsCaBr₃:Yb²⁺. Journal of Physics Condensed Matter, 2013, 25, 415504.	1.8	10
121	Ab Initio Calculations on Excited States of Lanthanide Containing Materials. Fundamental Theories of Physics, 2016, 50, 65-89.	0.3	10
122	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
123	Energy Shift of the 4f¹³6s¹Excited States of Yb²⁺from Gas Phase to the CsCaBr₃Solid. Spectroscopy Letters, 2010, 43, 393-399.	1.0	9
124	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
125	Energy level shifts in two-step spinâ€“orbit coupling ab initio calculations. Chemical Physics Letters, 2010, 498, 226-228.	2.6	8
126	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

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127	Extended model potential calculations on I2 and HI molecules. Journal of Chemical Physics, 1986, 84, 1941-1942.	3.0	7
128	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
129	Fine-Tuning the Cr³⁺ R₁-Line by Controlling Pauli Antisymmetry Strength. Journal of Physical Chemistry Letters, 2019, 10, 3176-3180.	4.6	6
130	Linear expansion of the eigenvalues of a Hermitian matrix and its application to the analysis of the electronic spectra of 3d ions in crystals. Journal of Solid State Chemistry, 1985, 56, 241-248.	2.9	5
131	Beyond the Embedded-Cluster Approximation: An ab initio Treatment of Polarization Effects. NATO ASI Series Series B: Physics, 1992, , 565-576.	0.2	5
132	Association of proteins: Adaptation and coupling of two available programs. Computer Physics Communications, 1986, 41, 169-177.	7.5	3
133	Recognition of amino acids in solution: The role of the hydrophobic forces. Journal of Biological Physics, 1986, 14, 107-111.	1.5	3
134	Basis sets generation: Relation between Adamowicz's and the maximum overlap method. International Journal of Quantum Chemistry, 1987, 31, 279-285.	2.0	3
135	Theoretical studies of transplantation antigens: Predicted conformation and structure-function relationship of the murine MHC class i antigen H-2Kb. Computational and Theoretical Chemistry, 1988, 179, 27-39.	1.5	3
136	Reduction of orbital sets. Computer Physics Communications, 1987, 43, 269-277.	7.5	2
137	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
138	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
139	Matrix linearization. Computer Physics Communications, 1986, 42, 127-136.	7.5	0
140	Ab initio calculations of lanthanide and Actinide Ions in Solids Using MOLCAS. , 2006, , 1307-1307.		0
141	Embedded-Cluster Calculations. , 1994, , 341-356.		0