Samir F Matar

List of Publications by Year
in descending order

344 papers	5,622 citations	108046 37 h-index	182931 54 g-index
390 all docs	390 docs citations	390 times ranked	5272 citing authors

#	Article	IF	Citations
1	First-principles investigations of tricarbon: From the isolated C3 molecule to a novel ultra-hard anisotropic solid. Carbon Trends, 2022, 6, 100132.	1.4	5
2	Novel trigonal BC11 as model structure of heavily-doped diamond: Crystal chemistry rationale and first principles characterizations. Diamond and Related Materials, 2022, 123, 108842.	1.8	2
3	Polymorphism of boron phosphide: theoretical investigation and experimental assessment. Journal of Materials Chemistry C, 2022, 10, 3937-3943.	2.7	8
4	Peierls distortion of the cobalt chain in the low-temperature structure of CoIn₂. Zeitschrift Fur Kristallographie - Crystalline Materials, 2022, 237, 239-248.	0.4	4
5	Novel ultra-hard hexacarbon allotropes from first principles. Solid State Sciences, 2022, 129, 106884.	1.5	2
6	The simplest dense carbon allotrope: Ultra-hard body-centered tetragonal C4. Journal of Solid State Chemistry, 2022, 314, 123424.	1.4	5
7	First-principles studies of the electronic and magnetic structures and bonding properties of boron subnitride B13N2. Journal of Solid State Chemistry, 2021, 294, 121840.	1.4	3
8	Charge transfer driven by ultrafast spin transition in a CoFe Prussian blue analogue. Nature Chemistry, 2021, 13, 10-14.	6.6	96
9	rh.-B12 as host of interstitial atoms: Review of a large family with illustrative study of B12{CN2} from first-principles. Progress in Solid State Chemistry, 2021, 61, 100296.	3.9	5
10	Electron Lone-Pairs Stereochemistry and Drastic van der Waals and Pressure Effects in AsF3 from First Principles. Condensed Matter, 2021, 6, 31.	0.8	2
11	Crystal chemistry and ab initio prediction of ultrahard rhombohedral B2N2 and BC2N. Solid State Sciences, 2021, 118, 106667.	1.5	13
12	Ultra-hard rhombohedral carbon by crystal chemistry and ab initio investigations. Journal of Solid State Chemistry, 2021, 302, 122354.	1.4	7
13	Crystal chemistry rationale and ab initio investigation of ultra-hard dense rhombohedral carbon and boron nitride. Diamond and Related Materials, 2021, 120, 108607.	1.8	6
14	Electronic and Magnetic Structures of New Interstitial Boron Sub-Oxides B12O2:X (X = B, C, N, O). Molecules, 2021, 26, 123.	1.7	3
15	Electronic structures of new layered hexaboron Crâ€“B compounds from first principles. Solid State Sciences, 2020, 99, 106069.	1.5	2
16	Diiron in extended carbon networks: Magnetic properties of model Fe2C6 and Fe2C12 from first principles. Journal of Magnetism and Magnetic Materials, 2020, 514, 167213.	1.0	2
17	C-2p Spin-Polarizations along with Two Mechanisms in Extended Carbon Multilayers: Insight from First Principles. Condensed Matter, 2020, 5, 48.	0.8	0
18	Se2TiO6E2 Ternary Oxide Characteristic of Isolated TiO6 Octahedra with the Shear Effect of SeIVE Electron Lone Pair (E): Combined Crystal Chemistry and ab Initio Study. Journal of Physical Chemistry C, 2020, 124, 12281-12285.	1.5	0

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19	Direct observation of nuclear reorganization driven by ultrafast spin transitions. Nature Communications, 2020, 11, 1530.	5.8	20
20	Electronic and magnetic properties of new binary uranium-boron compounds with 2D and 3D boron networks: A revisit of the U:B system. Solid State Sciences, 2020, 101, 106150.	1.5	2
21	Magnetization on nitrogen in extended honeycomb carbon layers from first principles: Case studies of CxN (xâ€¯=â€¯2, 6, 12). Journal of Magnetism and Magnetic Materials, 2019, 469, 46-51.	1.0	3
22	Nitrided FeNi: Chemical versus magnetovolume effects from ab initio. Journal of Magnetism and Magnetic Materials, 2019, 491, 165555.	1.0	1
23	Joint stereochemical and ab initio overview of SnII electron lone pairs (E) and Fâ¯(E) triplets effects on the crystal networks, the bonding and the electronic structures in a family of tin fluorides. Progress in Solid State Chemistry, 2019, 56, 100252.	3.9	3
24	Correlations of Crystal and Electronic Structure via NMR and X-ray Photoelectron Spectroscopies in the RETMAl₂ (RE = Sc, Y, Laâ€“Nd, Sm, Gdâ€“Tm, Lu; TM = Ni, Pd, Pt) Series. Inorganic Chemistry, 2019, 58, 7010-7025.	1.9	16
25	First principles investigation of magnetic new carbon-rich layered compounds UC (n= 2, 6, 12). Computational Condensed Matter, 2019, 21, e00397.	0.9	0
26	Cr2N2Se covalent ferromagnet proposed from first principles with properties close to CrO2. Solid State Sciences, 2019, 92, 53-59.	1.5	1
27	Electronic structure and magnetic ordering of NiN and Ni ₂ N from first principles. Electronic Structure, 2019, 1, 015002.	1.0	6
28	Coloring in the ZrBeSi-type structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2019, 74, 307-318.	0.3	14
29	Lattice phonon modes of the spin crossover crystal [Fe(phen)2(NCS)2] studied by THz, IR, Raman spectroscopies and DFT calculations. European Physical Journal B, 2019, 92, 1.	0.6	47
30	ZrNiAl-type gallides with pronounced metal-metal bonding, and the dimorphism of ScPdGa. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2019, 74, 15-25.	0.3	2
31	First principles investigations of Fe, Co, Ni in model honeycomb carbon networks. Solid State Sciences, 2019, 87, 155-162.	1.5	2
32	Impact of Spin State Transition on Vibrations of [Feâ€“(PMâ€“BiA)₂(NCS)₂] and [Feâ€“(PMâ€“PEA)₂(NCS)₂] Spin Crossover Compounds: Experimental and Theoretical Far IR and Raman Study. European Journal of Inorganic Chemistry, 2018, 2018, 385-393.	1.0	2
33	Rare earth-rich compounds RE9TMg4 (REÂ= Y, Dy-Tm, Lu; TÂ= Ru, Rh, Os, Ir) with an ordered Co2Al5-type structure. Solid State Sciences, 2018, 82, 70-77.	1.5	9
34	High pressure in solid state chemistry: Combined experimental and modeling approaches for assessing and predicting properties. Solid State Sciences, 2018, 80, 178-195.	1.5	1
35	The alkaline earth-palladium-germanides Sr3Pd4Ge4 and BaPdGe. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2018, 73, 243-250.	0.3	2
36	Electronic and Structural Dynamics During the Switching of the Photomagnetic Complex [Fe(L₂₂₂N₅)(CN)₂]. Chemistry - A European Journal, 2018, 24, 5064-5069.	1.7	13

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37	Two superstructures of Ce3Rh4Ge4. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 81-95.	0.4	2
38	Combined crystal chemistry and DFT studies of ThNCl and Th 2 N 2 X (X:Âchalcogen) behaving as pseudo-binaries. Solid State Sciences, 2018, 76, 1-7.	1.5	0
39	Chelating Mechanisms of Transition Metals by Bacterial Metallophores â€œPseudopaline and Staphylopineâ€: A Quantum Chemical Assessment. Computation, 2018, 6, 56.	1.0	11
40	Peculiar magnetic properties of NC6 and NC12 layered compounds from first principles. Journal of Theoretical and Applied Physics, 2018, 12, 209-217.	1.4	0
41	ns2 lone pair (E) and structural evolution of trichlorides M*Cl3E (M*Â= N, P, As, Sb and Bi) series. Stereochemistry and ab initio topology of Cl electron pair triplets. Solid State Sciences, 2018, 82, 44-51.	1.5	2
42	First Principles Study of Topochemical Effects and Electronic Structure Relationships between ANCl and A2N2Se (A = Zr, Ce) Assimilated to Pseudo-Binaries: {AN}Cl and {A2N2}Se. Computation, 2018, 6, 30.	1.0	1
43	Preface in memory of professor GÃ©rard Demazeau (June 8, 1943â€“November 3, 2017). Solid State Sciences, 2018, 82, A1-A3.	1.5	0
44	n s 2 n p 4 (n Â=Â4, 5) lone pair triplets whirling in M*F 2 E 3 (M*Â=ÂKr, Xe): Stereochemistry and ab initio analyses. Solid State Sciences, 2017, 64, 114-124.	1.5	5
45	Electronic structure and chemical bonding in LaIrSi-type intermetallics. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 207-213.	0.3	6
46	The nitridoborate nitrides Mg₃[BN₂]N and Ca₃[BN₂]N â€“ electronic structure and chemical bonding. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 433-439.	0.3	4
47	Coherent structural trapping through wave packet dispersion during photoinduced spin state switching. Nature Communications, 2017, 8, 15342.	5.8	149
48	Strong p -magnetism in carbon suboxide C 2 O devised from first principles. Chemical Physics Letters, 2017, 674, 115-119.	1.2	4
49	First-principles investigations of the electronic and magnetic structures and the bonding properties of uranium nitride fluoride (UNF). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 725-730.	0.3	1
50	(CaO) IrO2 (n = 1, 2, 4) family: Chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study. Journal of Solid State Chemistry, 2017, 255, 82-88.	1.4	10
51	Stereochemistry and ab initio topology analyses of electron lone pair triplets and twins in interhalogen compounds and halogen suboxides. Progress in Solid State Chemistry, 2017, 47-48, 1-18.	3.9	3
52	First principles studies of hydrogen insertion effects on magnetic properties, bonding and structure reordering of UZr 2. Computational Condensed Matter, 2017, 12, 19-24.	0.9	3
53	Stereochemistry of nitrogen E lone pair in NH3E, NOFE, N2O3E2, AgNO2E, and NCl3E. Comptes Rendus Chimie, 2017, 20, 446-459.	0.2	8
54	Activation of coherent lattice phonon following ultrafast molecular spin-state photo-switching: A molecule-to-lattice energy transfer. Structural Dynamics, 2016, 3, 023605.	0.9	28

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55	Electronic and magnetic structures and bonding properties of Ce 2 CrN 3 and U 2 CrN 3 from first principles. Computational Condensed Matter, 2016, 9, 13-18.	0.9	3
56	Drastic changes of electronic structure and crystal chemistry upon oxidation of SnII2TiO4E2 into SnIV2TiO6: An ab initio study. Solid State Sciences, 2016, 59, 25-31.	1.5	2
57	Quaternary Germanides RE₃TRh₄Ge₄ (RE = Ce,) Tj ETQq1 1 0.784314 rgBT Anorganische Und Allgemeine Chemie, 2016, 642, 979-986.	0.6	7
58	A ZrNiAl related high-pressure modification of CeRuSn. Dalton Transactions, 2016, 45, 14216-14229.	1.6	6
59	Ternary silicides ScIr₄Si₂ and RERh₄Si₂ (REâ€‰=â€‰Sc, Y, Tb-Lu) and quaternary derivatives RERh₄Si2â€“xSnx (REâ€‰=â€‰Y, Nd, Sm, Gd-Lu) â€“ structure, chemical bonding, and solid state NMR spectroscopy. Zeitschrift Fur Kristallographie - Crystalline Materials, 2016, 231, 475-486.	0.4	4
60	Unusual onset of p-element magnetization in a two dimensional structure. Solid State Sciences, 2016, 60, 55-58.	1.5	3
61	Lone electron pair (E) role on the crystal structures and the mechanism of high ionic conductivity of PbSnF 4 E 2 . Stereochemical and ab initio investigations. Solid State Sciences, 2016, 52, 29-36.	1.5	10
62	Ab initio proposition of novel BCN3 hard material based on the intergrowth of wurtzite and pyrite-like motifs. Computational Condensed Matter, 2016, 7, 14-19.	0.9	2
63	Tl(I) to Po(IV) 6s2 lone pairs in tetrahedral, triangular bipyramidal, square pyramidal, octahedral and hexahedral geometries: Crystal chemistry and ab initio visualizations and analyses. Progress in Solid State Chemistry, 2016, 44, 35-58.	3.9	9
64	Ab initio studies of the structural, electronic, and optical properties of quaternary B x Al y Ga1â€“xâ€“y N compounds. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 125-134.	0.3	4
65	Dimorphic HT- and LT-TbTiGe: Electronic and magnetic structures and bonding properties from first principles. Journal of Magnetism and Magnetic Materials, 2016, 397, 275-280.	1.0	0
66	Ultrafast Light-Induced Spin-State Trapping Photophysics Investigated in Fe(phen)₂(NCS)₂ Spin-Crossover Crystal. Accounts of Chemical Research, 2015, 48, 774-781.	7.6	85
67	Femtosecond spin-state photo-switching dynamics in an Fe^{III} spin crossover solid accompanied by coherent structural vibrations. Journal of Materials Chemistry C, 2015, 3, 7792-7801.	2.7	13
68	First principles investigation of the crystal and electronic structures of CeNCl and â€œCeNFâ€• Solid State Sciences, 2015, 48, 1-6.	1.5	2
69	Multiscale Experimental and Theoretical Investigations of Spin Crossover FeII Complexes: Examples of [Fe(phen)2(NCS)2] and [Fe(PM-BiA)2(NCS)2]. International Journal of Molecular Sciences, 2015, 16, 4007-4027.	1.8	16
70	Coherent view of crystal chemistry and ab initio analyses of Pb(II) and Bi(III) lone pair in square planar coordination. Progress in Solid State Chemistry, 2015, 43, 82-97.	3.9	21
71	LaMgX and CeMgX (XÂ=ÂGa, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure â€“ A systematic view on electronic structure and chemical bonding. Solid State Sciences, 2015, 43, 28-34.	1.5	3
72	Rhodium-rich germanides RERh4Ge2 (REÂ=ÂY, Gdâ€“Lu): structure and bonding. Monatshefte FÃ¼r Chemie, 2015, 146, 1375-1383.	0.9	5

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73	Chemical bonding in equiatomic cerium intermetallics â€“ The case of CeMgSn, CePdSn, and CeMgPb. Solid State Sciences, 2015, 48, 205-211.	1.5	2
74	Chemical bonding in RFe6Ge4 (RÂ=ÂLi, Sc, Zr) and LuTi6Sn4 with rhombohedral LiFe6Ge4 type structure. Solid State Sciences, 2015, 39, 82-91.	1.5	4
75	First principles account for large changes in electronic structure and bonding from LaCu to LaCuMg and LaCuMg4. Computational Materials Science, 2015, 97, 231-236.	1.4	0
76	Crystal and chemical anisotropy effects in AE2ZnN2, (AEÂ=ÂCa, Sr, Ba) from ab initio. Solid State Sciences, 2015, 39, 10-14.	1.5	3
77	Sequential Activation of Molecular Breathing and Bending during Spin-Crossover Photoswitching Revealed by Femtosecond Optical and X-Ray Absorption Spectroscopy. Physical Review Letters, 2014, 113, 227402.	2.9	115
78	Advanced Technologies for Produced Water Treatment. , 2014, , .		5
79	Ab-initio Studies of the Electronic Structures of the Hexavalent Uranium Compounds K₂UO₄ and Na₄UO₅. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 109-115.	0.3	0
80	The Silicides YT₂Si₂ (T =Co, Ni, Cu, Ru, Rh, Pd): A Systematic Study by ⁸⁹Y Solid-state NMR Spectroscopy. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 305-312.	0.3	11
81	Carbon-modified MgH2: Experimental and ab-initio Investigations. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 804-810.	0.3	1
82	Electronic Structure, Chemical Bonding and Electrochemical Characterization of Li2CuSn2 and Li2AgSn2. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 1010-1020.	0.3	2
83	The Gallium Intermetallics REPdGa₃ (RE=La, Ce, Pr, Nd, Sm, Eu) with SrPdGa₃-type Structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 1105-1118.	0.3	30
84	Drastic changes in the electronic and magnetic structures of hydrogenated U2Ti intermetallic from first principles. Journal of Magnetism and Magnetic Materials, 2014, 358-359, 70-75.	1.0	5
85	Electronic and magnetic structures and bonding properties of Ce2T2X (TÂ=Ând element; XÂ=ÂMg, Cd, Pb or) Tj ETQq1 1 0.784314 rg	1.8	9
86	Electronic structure and crystal phase stability of palladium hydrides. Journal of Applied Physics, 2014, 116, .	1.1	37
87	The Family of LiCo₆P₄ Type Compounds â€“ Trends in Electronic Structure and Chemical Bonding. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 1641-1647.	0.6	5
88	Ab initio study of MgH 2 : Destabilizing effects of selective substitutions by transition metals. Solid State Sciences, 2014, 36, 47-51.	1.5	5
89	Electronic structure and peculiar bonding properties of NdNiMg5 from first principles. Solid State Sciences, 2014, 38, 1-6.	1.5	5
90	Pressure induced metallization of fordite SnNb2O6 from first principles. Computational Materials Science, 2014, 84, 355-359.	1.4	3

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91	In silico CrNF, a half-metallic ferromagnetic nitrideâ€“fluoride mimicking CrO2. Journal of Magnetism and Magnetic Materials, 2014, 368, 105-110.	1.0	7
92	The U4Re7Si6 type â€“ Trends in electronic structure and chemical bonding. Solid State Sciences, 2014, 27, 5-10.	1.5	5
93	Drastic changes of electronic structure, bonding properties and crystal symmetry in Zr2Cu by hydrogenation, from ab initio. Intermetallics, 2014, 45, 5-10.	1.8	3
94	Kinetic Hydrate Inhibitor Removal by Physical, Chemical and Biological Processes. , 2014, , .		1
95	Kinetic Hydrate Inhibitor Removal by Physical, Chemical and Biological Processes. , 2014, , .		4
96	Linear infinite cadmium chains in CaAu4Cd2 and other intermetallics with YbMo2Al4-type structure. Monatshefte FÃ¼r Chemie, 2013, 144, 751-760.	0.9	19
97	Light elements-induced iono-covalent character in MgH2: An ab-initio approach. Computational Materials Science, 2013, 69, 424-427.	1.4	15
98	Ab initio investigations of the electronic and magnetic structures ofÂCoH and CoH2. Solid State Sciences, 2013, 22, 77-81.	1.5	7
99	First principles study of the electronic and magnetic structures and bonding properties of UCoC2 ternary, characteristic of Câ€“C units. Solid State Sciences, 2013, 17, 128-133.	1.5	1
100	Changes in electronic, magnetic and bonding properties from Zr2FeH5 to Zr3FeH7 addressed from ab initio. Solid State Sciences, 2013, 25, 55-62.	1.5	2
101	Molecular dynamics of spin crossover: The (P,T) phase diagram of [Fe(PM-BIA)2(NCS)2]. Chemical Physics, 2013, 420, 25-34.	0.9	10
102	The ternary germanides UMnGe and U2Mn3Ge. Solid State Sciences, 2013, 21, 73-80.	1.5	5
103	Drastic changes of electronic, magnetic, mechanical and bonding properties in Zr2Co by hydrogenation. Intermetallics, 2013, 36, 25-30.	1.8	9
104	Ab initio investigation of the crystal and electronic structures ofÂtheÂnitride fluoride ThNF. Solid State Sciences, 2013, 18, 123-126.	1.5	4
105	Electronic Structure and Bonding in YTi2Ga4 â€“ A Gallide with Linear Titanium Chains and Four-bonded Gallium Atoms. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2013, 68, 23-28.	0.3	10
106	CaTMg₂ and CaTCd₂ (T =Rh, Pd, Pt) with YPd₂Si-type Structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2013, 68, 111-120.	0.3	6
107	Change of the cerium valence with temperature â€“ Structure and chemical bonding of HT-CeRhGe. Solid State Sciences, 2013, 21, 6-10.	1.5	18
108	Review on cerium intermetallic compounds: A bird's eye outlook through DFT. Progress in Solid State Chemistry, 2013, 41, 55-85.	3.9	28

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109	Ab initio investigations of the electronic structures and chemical bonding in LiCo6P4 and Li2Co12P7. Journal of Solid State Chemistry, 2013, 202, 227-233.	1.4	4
110	Spin crossover complexes [Fe(NH2trz)3](X)2Â·nH2O investigated by means of polarized Raman scattering and DFT calculations. Physical Chemistry Chemical Physics, 2013, 15, 18128.	1.3	18
111	Drastic changes in electronic, magnetic, mechanical and bonding properties from Zr2CoH5 to Mg2CoH5. Journal of Solid State Chemistry, 2013, 200, 209-214.	1.4	5
112	ScPdZn and ScPtZn with YAlGe Type Structure â€“ Groupâ€“Subgroup Relation and ⁴⁵Sc Solid State NMR Spectroscopy. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 246-253.	0.6	6
113	Magnesium and Cadmium in Covalentlyâ€Bonded Lonsdaleite Networks: Synthesis, Structure, and Bonding of AETMg₂ and SrTCd₂ (AE = Ca, Sr; T = Pd,) Tj ETQq1 1 0.784314 rgBT	1.1	43
114	Single-crystal Data of Ternary Germanides RE2Nb3Ge4 (RE = Sc, Y, Gdâ€“Er, Lu) and Sc2Ta3Ge4 with Ordered Sm5Ge4-type Structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2013, 68, 625-634.	0.3	2
115	Hydrogen Insertion Effects on the Electronic Structure of Equiatomic MgNi Traced by ab initio Calculations. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2013, 68, 44-50.	0.3	2
116	Segregation of Calcium and Magnesium into Different Substructures. Ca₄Ag_{0.948}Mg and Other Compounds with Gd₄RhIn-type Structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2012, 67, 61-69.	0.3	24
117	Intermediate cerium valence intermetallics Ce4RuMg, Ce23Ru7Mg4, CeRu2Mg5, and Ce2Ru4Mg17: Electronic structures and chemical bonding from DFT. Intermetallics, 2012, 31, 88-93.	1.8	13
118	Transition metal hydrido-complexes: Electronic structure and bonding properties. Progress in Solid State Chemistry, 2012, 40, 31-40.	3.9	8
119	Underpinning energetics of lithium bonding and stability in the Liâ€“Ptâ€“Sn system. Solid State Sciences, 2012, 14, 1471-1475.	1.5	4
120	First principles investigations of the electronic structure and chemical bonding of U3Si2C2 â€“ A uranium silicideâ€“carbide with the rare [SiC] unit. Chemical Physics Letters, 2012, 550, 88-93.	1.2	5
121	Dimorphic LaPdSn and ErAgSn â€“ A first principles study. Intermetallics, 2012, 20, 33-38.	1.8	5
122	Electronic structure and chemical bonding of Li4Pt3Si. Chemical Physics Letters, 2012, 542, 47-51.	1.2	3
123	Solid-state 119Sn NMR and MÃ¨ssbauer Spectroscopic Studies of the Intermediate-valent Stannide CeRuSn. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2012, 67, 473-478.	0.3	9
124	Ab initio investigations of the electronic structure and lithium stability in Li2UN2 and LiUN2. Monatshefte FÃ¼r Chemie, 2012, 143, 1341-1348.	0.9	2
125	Ab initio investigation of the electronic structure of CeRh2Sb2. Chemical Physics Letters, 2012, 537, 48-52.	1.2	0
126	Electronic structure and anisotropic chemical bonding in TiNF from ab initio study. Journal of Solid State Chemistry, 2012, 185, 25-30.	1.4	6

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127	Electronic structure and chemical bonding of Î±- and Î²-CeIr2Si2 intermediate valence compounds. Journal of Solid State Chemistry, 2012, 186, 81-86.	1.4	5
128	Ab initio investigations of the electronic structure and chemical bonding of Li2ZrN2. Journal of Solid State Chemistry, 2012, 190, 191-195.	1.4	6
129	Electronic structure and chemical bonding of LiYSi. Solid State Sciences, 2012, 14, 375-380.	1.5	7
130	7Li and 29Si solid state NMR and chemical bonding of La2Li2Si3. Solid State Sciences, 2012, 14, 367-374.	1.5	10
131	Electronic structure and bonding of the hydrides Mg3TH7 (TÂ=ÂMn, Re) from first principles. Solid State Sciences, 2012, 14, 639-643.	1.5	2
132	The predominance of the rutile phase of SnO2 : First principles study. Solid State Communications, 2012, 152, 349-353.	0.9	6
133	New Quaternary Hydride CeZnSnH1.5: Structure, Magnetism, and Chemical Bonding. Chemistry of Materials, 2011, 23, 1096-1104.	3.2	10
134	Electronic properties of oxides: Chemical and theoretical approaches. Progress in Solid State Chemistry, 2011, 39, 70-95.	3.9	67
135	Drastic Change of the Ferromagnetic Properties of the Ternary Germanide GdTiGe through Hydrogen Insertion. Inorganic Chemistry, 2011, 50, 11046-11054.	1.9	24
136	First Principles Investigation of the Stability and the Chemical Behavior of Hydrogen in ThCoH4. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2011, 66, 269-274.	0.3	0
137	Ab initio investigations of the perovskite and K2NiF4 phases in the Csâ€“Caâ€“H system. Solid State Sciences, 2011, 13, 569-573.	1.5	3
138	Ab initio study of the hydrogenation effects on the electronic, chemical, and magnetic structures of CeIrSb. Solid State Sciences, 2011, 13, 948-952.	1.5	4
139	Crystal and electronic structure of LaPdSn and RE3Pd4Sn6 (REÂ=ÂLa, Ce). Solid State Sciences, 2011, 13, 1285-1290.	1.5	6
140	Ab initio investigations of the Ca2IrO4-type structure as a â€œpost-K2NiF4â€• Case study of Na2OsO4. Solid State Sciences, 2011, 13, 1396-1400.	1.5	8
141	First principles investigations of the hydrogenation effects on the electronic structure and the chemical bonding of CeIrAl. Solid State Sciences, 2011, 13, 1704-1708.	1.5	5
142	Nickel induced iono-covalent character of hydrogen in RbMgH3 from first principles. Chemical Physics Letters, 2011, 516, 174-176.	1.2	3
143	Palladium site ordering and the occurrence of superconductivity in Bi2Pd3Se2â^'xSx. Journal of Solid State Chemistry, 2011, 184, 797-804.	1.4	11
144	First principles study of Ca2PtO4 in K2NiF4 and â€˜post-K2NiF4â€™ type structures. Chemical Physics Letters, 2011, 503, 49-52.	1.2	2

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145	Electronic structure and equation of state of PdO2 from ab initio. Chemical Physics Letters, 2011, 508, 215-218.	1.2	21
146	SrAu_{4.76}In_{1.24} with YbMo₂Al₄-type Structure. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2011, 66, 993-999.	0.3	8
147	Effect of the Ball Milling Conditions, under Air, on the Preliminary Hydriding Properties of the Mixtures Mg-x Wt% Graphite. Role of Solvent. Advanced Materials Research, 2011, 324, 119-124.	0.3	4
148	From antiferromagnetic to ferromagnetic ordering induced by hydrogenation of the compounds NdCoSi and NdCoGe. Journal of Physics: Conference Series, 2010, 200, 032012.	0.3	6
149	Intermetallic hydrides: A review with ab initio aspects. Progress in Solid State Chemistry, 2010, 38, 1-37.	3.9	80
150	YNi and its hydrides: Phase stabilities, electronic structures and chemical bonding properties from first principles. Chemical Physics, 2010, 377, 109-114.	0.9	4
151	La6Pd13Cd4 and Ce6Pd13Cd4 with palladium-centred rare earth octahedra: synthesis, structure, and chemical bonding. Monatshefte FÃ¼r Chemie, 2010, 141, 1-6.	0.9	4
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