Antoine Villesuzanne

List of Publications by Citations

44 papers	818 citations	17 h-index	28 g-index
55 ext. papers	928 ext. citations	4.7 avg, IF	3.62 L-index

#	Paper	IF	Citations
44	Rapid hydrothermal synthesis of VO2 (B) and its conversion to thermochromic VO2 (M1). *Inorganic Chemistry*, **2013**, 52, 4780-5	5.1	88
43	Application of Density Functional Theory to the Modeling of the Mixed Ionic and Electronic Conductor La2NiO4+ Lattice Relaxation, Oxygen Mobility, and Energetics of Frenkel Defects. *Chemistry of Materials*, **2005**, 17, 6538-6544	9.6	67
42	LiMSO(4)F (M = Fe, Co and Ni): promising new positive electrode materials through the DFT microscope. *Physical Chemistry Chemical Physics*, **2010**, 12, 15512-22	3.6	59
41	Anisotropic Oxygen Diffusion Properties in Pr2NiO4+and Nd2NiO4+Single Crystals. *Journal of Physical Chemistry C*, **2013**, 117, 26466-26472	3.8	58
40	Determination of Local Geometries around Tellurium in TeO2Nb2O5and TeO2Al2O3Oxide Glasses by XANES and EXAFS: Investigation of Electronic Properties of Evidenced Oxygen Clusters byAb InitioCalculations. *Journal of Solid State Chemistry*, **1996**, 126, 143-151	3.3	51
39	VO2 (A): Reinvestigation of crystal structure, phase transition and crystal growth mechanisms. *Journal of Solid State Chemistry*, **2014**, 213, 79-86	3.3	46
38	Spin State Behavior in Some Cobaltites (III) and (IV) with Perovskite or Related Structure. *Journal of Solid State Chemistry*, **2001**, 162, 282-292	3.3	42
37	Density functional theory calculations on microscopic aspects of oxygen diffusion in ceria-based materials. *International Journal of Quantum Chemistry*, **2005**, 101, 826-839	2.1	36
36	Synthesis, crystal structure, magnetic properties, and electronic structure of the new ternary vanadate CuMnVO4. *Inorganic Chemistry*, **2005**, 44, 3087-93	5.1	28
35	On the role of lattice dynamics on low-temperature oxygen mobility in solid oxides: a neutron diffraction and first-principles investigation of ({hbox{L}}{{hbox{a}}_2}{hbox{Cu}}{{hbox{O}}_{{4 + delta }}}). *Journal of Solid State Electrochemistry*, **2011**, 15, 357-366	2.6	26
34	Identifying Doping Strategies To Optimize the Oxide Ion Conductivity in Ceria-Based Materials. *Journal of Physical Chemistry C*, **2010**, 114, 19062-19076	3.8	26
33	New considerations on the role of covalency in ferroelectric niobates and tantalates. *European Physical Journal B*, **1998**, 6, 307-312	1.2	26
32	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 11398-412	3.6	22
31	First-principles study of the electronic and magnetic structures of the tetragonal and orthorhombic phases of Ca3Mn2O7. *Physical Review B*, **2007**, 76,	3.3	20
30	Density functional theory analysis of the interplay between Jahn-Teller instability, uniaxial magnetism, spin arrangement, metal-metal interaction, and spin-orbit coupling in Ca3CoMO6 (M = Co, Rh, Ir). *Inorganic Chemistry*, **2011**, 50, 1758-66	5.1	19
29	Synthesis and characterization of [PtIn6](GeO4)2O and its solid solution [PtIn6](GaO4)(2-x)(GeO4)xOx/2 (0 Journal of the American Chemical Society, **2005**, 127, 12990-6	16.4	18
28	Comparative Studies on the Phase Stability, Electronic Structure, and Topology of the Charge Density in the Li3XO4 (X = P, As, V) Lithium Orthosalt Polymorphs. *Chemistry of Materials*, **2009**, 21, 1861-1874	9.6	17

27	First-principles determination of structural properties of MgO. *Physica Scripta*, **2009**, 80, 055702	2.6	17
26	Comparative electronic band structure study of the intrachain ferromagnetic versus antiferromagnetic coupling in the magnetic oxides Ca3Co2O6 and Ca3FeRhO6. *Inorganic Chemistry*, **2005**, 44, 6339-45	5.1	17
25	Interplay between Local Electronic Configuration and the Occurrence of a Metallic State: An Experimental Approach. *Journal of Solid State Chemistry*, **1999**, 147, 211-217	3.3	16
24	(Nd/Pr)NiO: Reaction Intermediates and Redox Behavior Explored by in Situ Neutron Powder Diffraction during Electrochemical Oxygen Intercalation. *Inorganic Chemistry*, **2018**, 57, 4657-4666	5.1	13
23	Molecular-dynamics simulations of binary Pd-Si metal alloys: Glass formation, crystallisation and cluster properties. *Journal of Non-Crystalline Solids*, **2018**, 487, 72-86	3.9	12
22	Analysis of the effect of spin-orbit coupling on the electronic structure and excitation spectrum of the Bi2(2-) anion in (K-crypt)2Bi2 on the basis of relativistic electronic structure calculations. *Journal of Physical Chemistry A*, **2005**, 109, 1675-83	2.8	12
21	Ionic conductivity, ferroelectricity and chemical bonding in TKWB type ceramics of the K6Li4Ta10O30-Pb5Ta10O30 system. *Journal of Materials Chemistry*, **1998**, 8, 2423-2428		8
20	The electronic and magnetic structures of stoichiometric SrCoO3: ASW calculations. *Journal of Materials Chemistry*, **1996**, 6, 1785		8
19	Rippled nanocarbons from periodic arrangements of reordered bivacancies in graphene or nanotubes. *Journal of Chemical Physics*, **2012**, 136, 124705	3.9	7
18	Isolating the Two Room-Temperature Polymorphs of NaNbO3: Structural Features, Optical Band Gap, and Reactivity. *ACS Applied Electronic Materials*, **2019**, 1, 513-522	4	6
17	Long-range oxygen ordering linked to topotactic oxygen release in Pr2NiO4+□ fuel cell cathode material. *Journal of Materials Chemistry A*, **2020**, 8, 13987-13995	13	5
16	Status of trivalent copper and charge-transfer excitons in high-TC cuprates. *Inorganic Chemistry*, **2008**, 47, 8487-97	5.1	5
15	Large Negative Magnetoresistance of the Rare-Earth Transition-Metal Intermetallic Compound PrMnSi2. *Chemistry of Materials*, **2005**, 17, 6338-6341	9.6	5
14	Prediction of ferroelectric properties in niobates and tantalates based on covalency considerations. *Ferroelectrics*, **1999**, 229, 1-10	0.6	5
13	Discussion on the structure stability and the luminescence switch under irradiation of a Ce-doped elpasolite compound. *Chemistry - A European Journal*, **2015**, 21, 5242-51	4.8	4
12	On the Electronic Structure Required for the Uniaxial Magnetic Properties of the Magnetic Metal SrCo6O11. *Chemistry of Materials*, **2007**, 19, 2712-2714	9.6	4
11	Exchange and correlation effects in transition-metal oxides 3dn´(n = 4, 5 and 6). *Comptes Rendus Chimie*, **2003**, 6, 135-145	2.7	4
10	Hydrogen Insertion in the Intermetallic GdScGe: A Drastic Reduction of the Dimensionality of the Magnetic and Transport Properties. *Inorganic Chemistry*, **2018**, 57, 14230-14239	5.1	4

9	Effect of Carbon Insertion on the Structural and Magnetic Properties of NdScSi. *Inorganic Chemistry* , **2019**, 58, 15255-15268	5.1	3
8	High-TC superconductivity: a solid state chemistry model. *New Journal of Chemistry*, **2012**, 36, 796	3.6	3
7	Real-space pairing through charge transfer excitons in high-TC cuprates. *Inorganic Chemistry*, **2008**, 47, 11958-64	5.1	3
6	Discussion on the structural anisotropy of wurtzite-type compounds. *Solid State Sciences*, **2013**, 21, 81-84	3.4	2
5	Solid state chemistry for connecting the pieces of the high-TC superconducting puzzle?. *Solid State Sciences*, **2010**, 12, 691-698	3.4	2
4	Observation of Unusual Hysteretic Magnetic Properties of the Rare Earth Intermetallic Compound PrMnSi2: Magnetic Susceptibility, Magnetization, Heat Capacity, and Electronic Band Structure Studies. *Chemistry of Materials*, **2005**, 17, 3711-3716	9.6	2
3	Etude des structures électroniques de In2O3 pur et dopé avec l'étain. *Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry*, **2001**, 4, 367-373		1
2	Are Superconductivity Mechanisms a Matter for Chemists?. *Condensed Matter*, **2020**, 5, 67	1.8	
1	A Density Functional Study of Oxygen Mobility in Ceria-Based Materials. *Defect and Diffusion Forum* , **2012**, 323-325, 233-238	0.7	