Pascal Boulet

List of Publications by Year
in descending order

82 papers	1,858 citations	279701 23 h-index	276775 41 g-index
85 all docs	85 docs citations	85 times ranked	2432 citing authors

#	Article	IF	Citations
1	Preparation and Chromaticity Control of CoTiO3/NiTiO3 Co-Coated TiO2 Composite Pigments. Materials, 2022, 15, 1456.	1.3	3
2	Electron Density and Optoelectronic Properties of Copper Antimony Sulphur Ternary Compounds for Photovoltaic Applications. Journal of Electronic Materials, 2022, 51, 3903-3918.	1.0	5
3	Influence of the stacking sequence on layered-chalcogenide properties: first principles investigation of Pb₂Bi₂Te₅. Physical Chemistry Chemical Physics, 2021, 23, 11300-11313.	1.3	5
4	Thermoelectric properties of Cuâ€Sb system compounds from density functional theory calculations. Journal of the Chinese Chemical Society, 2021, 68, 1030.	0.8	1
5	Strain Effects on the Electronic and Thermoelectric Properties of n(PbTe)-m(Bi2Te3) System Compounds. Materials, 2021, 14, 4086.	1.3	6
6	Structureâ€“Property Relationships in Transition Metal Dichalcogenide Bilayers under Biaxial Strains. Nanomaterials, 2021, 11, 2639.	1.9	4
7	First-Principle Investigations on the Electronic and Transport Properties of PbBi2Te2X2 (X=S/Se/Te) Monolayers. Nanomaterials, 2021, 11, 2979.	1.9	0
8	Thermoelectric Properties of Sb-S System Compounds from DFT Calculations. Materials, 2020, 13, 4707.	1.3	4
9	Structure-Property Relationships of 2D Ga/In Chalcogenides. Nanomaterials, 2020, 10, 2188.	1.9	2
10	Electron Density and Its Relation with Electronic and Optical Properties in 2D Mo/W Dichalcogenides. Nanomaterials, 2020, 10, 2221.	1.9	11
11	Theoretical Investigations of the BaRh2Ge4X6 (X = S, Se, Te) Compounds. Energies, 2020, 13, 6434.	1.6	0
12	A rapid method for analyzing the chemical bond from energy densities calculations at the bond critical point. Computational and Theoretical Chemistry, 2020, 1178, 112784.	1.1	29
13	First-principles calculations on CuInSe₂/AlP heterostructures. Journal of Materials Chemistry C, 2020, 8, 4732-4742.	2.7	7
14	New insight into the structure-property relationships from chemical bonding analysis: Application to thermoelectric materials. Journal of Solid State Chemistry, 2020, 286, 121266.	1.4	11
15	Stability Investigation of Se- and Te-Substituted Tetrahedrite. Journal of Electronic Materials, 2020, 49, 3566-3576.	1.0	1
16	Atomic bonding and electronic stability of the binary sigma phase. Journal of Alloys and Compounds, 2019, 811, 152053.	2.8	7
17	A DFT study of the electronic, optical and topological properties of free and biaxially strained CuIn_{1â^'x}Al_xSe₂. Journal of Materials Chemistry C, 2019, 7, 5803-5815.	2.7	14
18	Influence of atomic mixing and atomic order on molar volume of the binary sigma phase. Intermetallics, 2018, 98, 95-105.	1.8	4

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19	Influence of atomic order on the enthalpy of formation and bulk modulus of the sigma phase. Fluid Phase Equilibria, 2018, 459, 238-243.	1.4	6
20	Influence of nearest neighbor atoms and coordination polyhedron on atomic volume of sigma phases. Computational Materials Science, 2018, 143, 308-315.	1.4	3
21	Influencing factors of atomic order in the binary sigma phase. Intermetallics, 2018, 93, 6-19.	1.8	8
22	Oleylamine-assisted solvothermal synthesis of copper antimony sulfide nanocrystals: Morphology and phase control. Materials Research Bulletin, 2017, 90, 188-194.	2.7	7
23	Modeling of adsorption of CO2 in the deformed pores of MIL-53(Al). Journal of Molecular Modeling, 2017, 23, 101.	0.8	9
24	Strain-induced electronic band convergence: effect on the Seebeck coefficient of Mg2Si for thermoelectric applications. Journal of Molecular Modeling, 2017, 23, 130.	0.8	7
25	Heterogeneous melting of methane confined in nano-pores. Journal of Chemical Physics, 2016, 145, 144704.	1.2	8
26	Low temperature mechanism of adsorption of methane: Comparison between homogenous and heterogeneous pores. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 496, 86-93.	2.3	11
27	Simulation of liquidâ€“liquid interfaces in porous media. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 496, 28-38.	2.3	6
28	Polycrystalline Mg2Si thin films: A theoretical investigation of their electronic transport properties. Journal of Solid State Chemistry, 2015, 225, 174-180.	1.4	5
29	Thermoelectric Properties of Sn-Containing Mg2Si Nanostructures. Journal of Physical Chemistry C, 2015, 119, 17515-17521.	1.5	5
30	Efficiency assessment of novel materials based flexible thermoelectric devices by a multiscale modeling approach. Computational Materials Science, 2015, 108, 264-269.	1.4	8
31	Inserting Tin or Antimony Atoms into Mg2Si: Effect on the Electronic and Thermoelectric Properties. Journal of Electronic Materials, 2015, 44, 4452-4464.	1.0	5
32	Calculations of thermoelectric properties: Mg2Si under uniaxial [110] strains versus (110)-oriented thin film. European Physical Journal B, 2015, 88, 1.	0.6	4
33	Electronic and transport properties of Mg2Si under isotropic strains. Intermetallics, 2014, 50, 8-13.	1.8	20
34	Substitutional Atom Influence on the Electronic and Transport Properties of Mn4Si7. Journal of Electronic Materials, 2014, 43, 761-773.	1.0	10
35	DFT calculations of electronic and transport properties of substituted Mn4Si7. Journal of Alloys and Compounds, 2014, 584, 279-288.	2.8	15
36	Thermoelectric Properties of Mg₂Si Thin Films by Computational Approaches. Journal of Physical Chemistry C, 2014, 118, 19635-19645.	1.5	24

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37	Linear Thermal Expansion Coefficients of Higher Manganese Silicide Compounds. Physics Procedia, 2014, 55, 24-29.	1.2	10
38	Computational Investigation of the Electronic and Thermoelectric Properties of Strained Bulk Mg2Si. Journal of Electronic Materials, 2014, 43, 3801-3807.	1.0	7
39	Investigation of New Routes for the Synthesis of Mn4Si7. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 1645-1650.	1.1	5
40	Phase formation in Mnâ€“Si thin films during rapid thermal annealing. Intermetallics, 2013, 37, 69-75.	1.8	5
41	Phase transformations in Higher Manganese Silicides. Journal of Alloys and Compounds, 2013, 551, 30-36.	2.8	24
42	Mechanism of adsorption of p-cresol uremic toxin into faujasite zeolites in presence of water and sodium cations â€“ A Monte Carlo study. Microporous and Mesoporous Materials, 2013, 173, 70-77.	2.2	13
43	Grand canonical monte carlo modeling of hydrogen adsorption on phosphorus-doped open carbon framework. Adsorption, 2013, 19, 869-877.	1.4	6
44	Effect of Biaxial Strain on Electronic and Thermoelectric Properties of Mg2Si. Journal of Electronic Materials, 2013, 42, 3458-3466.	1.0	17
45	Computational investigation of the adsorption of carbon dioxide onto zirconium oxide clusters. Journal of Molecular Modeling, 2012, 18, 4819-4830.	0.8	10
46	Hypothetical High-Surface-Area Carbons with Exceptional Hydrogen Storage Capacities: Open Carbon Frameworks. Journal of the American Chemical Society, 2012, 134, 15130-15137.	6.6	66
47	Low-dimensional materials for thermoelectric applications. International Journal of Nanotechnology, 2012, 9, 368.	0.1	2
48	Adsorption of Carbon Dioxide on Mesoporous Zirconia: Microcalorimetric Measurements, Adsorption Isotherm Modeling, and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2011, 115, 10097-10103.	1.5	43
49	Electronic properties of the Mg2Si thermoelectric material investigated by linear-response density-functional theory. Computational Materials Science, 2011, 50, 847-851.	1.4	46
50	Electronic properties of Zn1â^'xCdxSb solid solution investigated by density-functional theory. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 639-642.	0.7	0
51	Dielectric, magnetic, and phonon properties of nickel hydroxide. Physical Review B, 2011, 84, .	1.1	99
52	Influence of the modified Becke-Johnson exchange potential on thermoelectric properties: Application to Mg2Si. Journal of Chemical Physics, 2011, 135, 234702.	1.2	26
53	Structural investigation of the Zn1â^'xCdxSb solid solution by density-functional theory approach. Solid State Sciences, 2010, 12, 26-32.	1.5	6
54	Adsorption of paracresol in silicalite-1 and pure silica faujasite. A comparison study using molecular simulation. Applied Surface Science, 2010, 256, 5470-5474.	3.1	5

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55	Adsorption into the MFI zeolite of aromatic molecule of biological relevance. Investigations by Monte Carlo simulations. Journal of Molecular Modeling, 2009, 15, 573-579.	0.8	7
56	Molecular Simulations of Water and Paracresol in MFI Zeolite - A Monte Carlo Study. Langmuir, 2009, 25, 11598-11607.	1.6	12
57	Modeling of adsorption in pores with strongly heterogeneous walls: parametric lattice-site wall model. Adsorption, 2008, 14, 201-205.	1.4	4
58	Adsorption of small uremic toxin molecules on MFI type zeolites from aqueous solution. Adsorption, 2008, 14, 377-387.	1.4	38
59	A critical appraisal of polymerâ€“clay nanocomposites. Chemical Society Reviews, 2008, 37, 568-594.	18.7	369
60	Microscopic Mechanism of Adsorption in Cylindrical Nanopores with Heterogenous Wall Structure. Langmuir, 2008, 24, 4013-4019.	1.6	21
61	Gaining Insight into the Structure and Dynamics of Clayâ€“Polymer Nanocomposite Systems Through Computer Simulation. , 2008, , 175-203.		0
62	Large-scale simulations of poly(propylene oxide)amine/Na+-montmorillonite and poly(propylene oxide) ammonium/Na+-montmorillonite using a molecular dynamics approach. Studies in Surface Science and Catalysis, 2007, , 311-318.	1.5	0
63	Adsorption of small uremic toxin molecules onto zeolites: a first step towards an alternative kidney. Studies in Surface Science and Catalysis, 2007, 170, 1015-1020.	1.5	6
64	Adsorption in cylindrical pores: Mixed lattice-site/off-site Monte Carlo simulations in pores with heterogeneous wall structure. Applied Surface Science, 2007, 253, 5596-5600.	3.1	13
65	Melting mechanism of monolayers adsorbed in cylindrical pores: An influence of the pore wall roughness. Applied Surface Science, 2007, 253, 5601-5605.	3.1	4
66	Adsorption of the uremic toxin p-cresol onto hemodialysis membranes and microporous adsorbent zeolite silicalite. Journal of Biotechnology, 2006, 123, 164-173.	1.9	51
67	Intercalation and in situ polymerization of poly(alkylene oxide) derivatives within M+-montmorillonite (M = Li, Na, K). Journal of Materials Chemistry, 2006, 16, 1082.	6.7	45
68	Recent advances in understanding the structure and reactivity of clays using electronic structure calculations. Computational and Theoretical Chemistry, 2006, 762, 33-48.	1.5	77
69	Morphology and elastic modulus of novel poly[oligo(ethylene glycol) diacrylate]-montmorillonite nanocomposites. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 1785-1793.	2.4	9
70	Interlayer Structure and Bonding in Nonswelling Primary Amine Intercalated Clays. Macromolecules, 2005, 38, 6189-6200.	2.2	73
71	Simulation of hydrated Li+-, Na+- and K+-montmorillonite/polymer nanocomposites using large-scale molecular dynamics. Chemical Physics Letters, 2004, 389, 261-267.	1.2	45
72	Understanding the Formation of New Clusters of Alkali and Alkaline Earth Metals:Â A New Synthetic Approach, Single-Crystal Structures, and Theoretical Calculations. Journal of the American Chemical Society, 2003, 125, 3593-3604.	6.6	35

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73	Combined experimental and theoretical investigations of clayâ€“polymer nanocomposites: intercalation of single bifunctional organic compounds in Na+-montmorillonite and Na+-hectorite clays for the design of new materials. Journal of Materials Chemistry, 2003, 13, 2540-2550.	6.7	55
74	Oxidation of Methanol to Formaldehyde Catalyzed by V2O5. A Density Functional Theory Study. Journal of Physical Chemistry B, 2002, 106, 9659-9667.	1.2	23
75	DFT Investigation of Metal Complexes Containing a Nitrosyl Ligand. 1. Ground State and Metastable States. Journal of Physical Chemistry A, 2001, 105, 8991-8998.	1.1	37
76	DFT Investigation of Metal Complexes Containing a Nitrosyl Ligand. 2. Excited States. Journal of Physical Chemistry A, 2001, 105, 8999-9003.	1.1	34
77	Photochemistry of the CpNiNO Complex. A Theoretical Study Using Density Functional Theory. Inorganic Chemistry, 2001, 40, 7032-7039.	1.9	21
78	Absorption Spectra of Several Metal Complexes Revisited by the Time-Dependent Density-Functional Theory-Response Theory Formalism. Journal of Physical Chemistry A, 2001, 105, 885-894.	1.1	96
79	Absorption and emission spectroscopy of matrix-isolated benzo[g,h,i]perylene: An experimental and theoretical study for astrochemical applications. Journal of Chemical Physics, 2001, 115, 1769-1776.	1.2	23
80	Reply to Comment on â€œTheoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by â€•[Chem. Phys. 253 (2000) 389â€“390]. Chemical Physics, 2000, 253, 391-392.	0.9	0
81	Density Functional Theory Calculations of the Oxidative Dehydrogenation of Propane on the (010) Surface of V2O5â€. Journal of Physical Chemistry B, 2000, 104, 12250-12255.	1.2	74
82	Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by H3+. Chemical Physics, 1999, 244, 163-174.	0.9	21