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	A critical appraisal of polymerâ€“clay nanocomposites. Chemical Society Reviews, 2008, 37, 568-594.	18.7	369
2	Dielectric, magnetic, and phonon properties of nickel hydroxide. Physical Review B, 2011, 84, .	1.1	99
3	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
4	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
5	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
6	Interlayer Structure and Bonding in Nonswelling Primary Amine Intercalated Clays. Macromolecules, 2005, 38, 6189-6200.	2.2	73
7	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
8	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
9	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
10	Electronic properties of the Mg2Si thermoelectric material investigated by linear-response density-functional theory. Computational Materials Science, 2011, 50, 847-851.	1.4	46
11	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
12	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
13	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
14	Adsorption of small uremic toxin molecules on MFI type zeolites from aqueous solution. Adsorption, 2008, 14, 377-387.	1.4	38
15	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
16	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
17	DFT Investigation of Metal Complexes Containing a Nitrosyl Ligand. 2. Excited States. Journal of Physical Chemistry A, 2001, 105, 8999-9003.	1.1	34
18	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

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19	Influence of the modified Becke-Johnson exchange potential on thermoelectric properties: Application to Mg2Si. Journal of Chemical Physics, 2011, 135, 234702.	1.2	26
20	Phase transformations in Higher Manganese Silicides. Journal of Alloys and Compounds, 2013, 551, 30-36.	2.8	24
21	Thermoelectric Properties of Mg₂Si Thin Films by Computational Approaches. Journal of Physical Chemistry C, 2014, 118, 19635-19645.	1.5	24
22	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
23	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
24	Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by H3+. Chemical Physics, 1999, 244, 163-174.	0.9	21
25	Photochemistry of the CpNiNO Complex. A Theoretical Study Using Density Functional Theory. Inorganic Chemistry, 2001, 40, 7032-7039.	1.9	21
26	Microscopic Mechanism of Adsorption in Cylindrical Nanopores with Heterogenous Wall Structure. Langmuir, 2008, 24, 4013-4019.	1.6	21
27	Electronic and transport properties of Mg2Si under isotropic strains. Intermetallics, 2014, 50, 8-13.	1.8	20
28	Effect of Biaxial Strain on Electronic and Thermoelectric Properties of Mg2Si. Journal of Electronic Materials, 2013, 42, 3458-3466.	1.0	17
29	DFT calculations of electronic and transport properties of substituted Mn4Si7. Journal of Alloys and Compounds, 2014, 584, 279-288.	2.8	15
30	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
31	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
32	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
33	Molecular Simulations of Water and Paracresol in MFI Zeolite - A Monte Carlo Study. Langmuir, 2009, 25, 11598-11607.	1.6	12
34	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
35	Electron Density and Its Relation with Electronic and Optical Properties in 2D Mo/W Dichalcogenides. Nanomaterials, 2020, 10, 2221.	1.9	11
36	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

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37	Computational investigation of the adsorption of carbon dioxide onto zirconium oxide clusters. Journal of Molecular Modeling, 2012, 18, 4819-4830.	0.8	10
38	Substitutional Atom Influence on the Electronic and Transport Properties of Mn4Si7. Journal of Electronic Materials, 2014, 43, 761-773.	1.0	10
39	Linear Thermal Expansion Coefficients of Higher Manganese Silicide Compounds. Physics Procedia, 2014, 55, 24-29.	1.2	10
40	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
41	Modeling of adsorption of CO2 in the deformed pores of MIL-53(Al). Journal of Molecular Modeling, 2017, 23, 101.	0.8	9
42	Efficiency assessment of novel materials based flexible thermoelectric devices by a multiscale modeling approach. Computational Materials Science, 2015, 108, 264-269.	1.4	8
43	Heterogeneous melting of methane confined in nano-pores. Journal of Chemical Physics, 2016, 145, 144704.	1.2	8
44	Influencing factors of atomic order in the binary sigma phase. Intermetallics, 2018, 93, 6-19.	1.8	8
45	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
46	Computational Investigation of the Electronic and Thermoelectric Properties of Strained Bulk Mg2Si. Journal of Electronic Materials, 2014, 43, 3801-3807.	1.0	7
47	Oleylamine-assisted solvothermal synthesis of copper antimony sulfide nanocrystals: Morphology and phase control. Materials Research Bulletin, 2017, 90, 188-194.	2.7	7
48	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
49	Atomic bonding and electronic stability of the binary sigma phase. Journal of Alloys and Compounds, 2019, 811, 152053.	2.8	7
50	First-principles calculations on CuInSe₂/AlP heterostructures. Journal of Materials Chemistry C, 2020, 8, 4732-4742.	2.7	7
51	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
52	Structural investigation of the Zn1â^'xCdxSb solid solution by density-functional theory approach. Solid State Sciences, 2010, 12, 26-32.	1.5	6
53	Grand canonical monte carlo modeling of hydrogen adsorption on phosphorus-doped open carbon framework. Adsorption, 2013, 19, 869-877.	1.4	6
54	Simulation of liquidâ€“liquid interfaces in porous media. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 496, 28-38.	2.3	6

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55	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
56	Strain Effects on the Electronic and Thermoelectric Properties of n(PbTe)-m(Bi2Te3) System Compounds. Materials, 2021, 14, 4086.	1.3	6
57	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
58	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
59	Phase formation in Mnâ€“Si thin films during rapid thermal annealing. Intermetallics, 2013, 37, 69-75.	1.8	5
60	Polycrystalline Mg2Si thin films: A theoretical investigation of their electronic transport properties. Journal of Solid State Chemistry, 2015, 225, 174-180.	1.4	5
61	Thermoelectric Properties of Sn-Containing Mg2Si Nanostructures. Journal of Physical Chemistry C, 2015, 119, 17515-17521.	1.5	5
62	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
63	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
64	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
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	Modeling of adsorption in pores with strongly heterogeneous walls: parametric lattice-site wall model. Adsorption, 2008, 14, 201-205.	1.4	4
67	Calculations of thermoelectric properties: Mg2Si under uniaxial [110] strains versus (110)-oriented thin film. European Physical Journal B, 2015, 88, 1.	0.6	4
68	Influence of atomic mixing and atomic order on molar volume of the binary sigma phase. Intermetallics, 2018, 98, 95-105.	1.8	4
69	Thermoelectric Properties of Sb-S System Compounds from DFT Calculations. Materials, 2020, 13, 4707.	1.3	4
70	Structureâ€“Property Relationships in Transition Metal Dichalcogenide Bilayers under Biaxial Strains. Nanomaterials, 2021, 11, 2639.	1.9	4
71	Influence of nearest neighbor atoms and coordination polyhedron on atomic volume of sigma phases. Computational Materials Science, 2018, 143, 308-315.	1.4	3
72	Preparation and Chromaticity Control of CoTiO3/NiTiO3 Co-Coated TiO2 Composite Pigments. Materials, 2022, 15, 1456.	1.3	3

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73	Low-dimensional materials for thermoelectric applications. International Journal of Nanotechnology, 2012, 9, 368.	0.1	2
74	Structure-Property Relationships of 2D Ga/In Chalcogenides. Nanomaterials, 2020, 10, 2188.	1.9	2
75	Stability Investigation of Se- and Te-Substituted Tetrahedrite. Journal of Electronic Materials, 2020, 49, 3566-3576.	1.0	1
76	Thermoelectric properties of Cuâ€Sb system compounds from density functional theory calculations. Journal of the Chinese Chemical Society, 2021, 68, 1030.	0.8	1
77	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
78	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
79	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
80	Theoretical Investigations of the BaRh2Ge4X6 (X = S, Se, Te) Compounds. Energies, 2020, 13, 6434.	1.6	0
81	First-Principle Investigations on the Electronic and Transport Properties of PbBi2Te2X2 (X=S/Se/Te) Monolayers. Nanomaterials, 2021, 11, 2979.	1.9	0
82	Gaining Insight into the Structure and Dynamics of Clayâ€“Polymer Nanocomposite Systems Through Computer Simulation. , 2008, , 175-203.		0