Bernard Delley

List of Publications by Citations

80 papers	5,284 citations	36 h-index	72 g-index
87 ext. papers	5,578 ext. citations	4 avg, IF	5.49 L-index

#	Paper	IF	Citations
80	Fast Calculation of Electrostatics in Crystals and Large Molecules. *The Journal of Physical Chemistry*, **1996**, 100, 6107-6110		747
79	Kondo Scattering Observed at a Single Magnetic Impurity. *Physical Review Letters*, **1998**, 80, 2893-2896	7.4	516
78	The generation and use of delocalized internal coordinates in geometry optimization. *Journal of Chemical Physics*, **1996**, 105, 192-212	3.9	264
77	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. *Physical Review B*, **2007**, 75,	3.3	247
76	Dissociation of O2 at Al(111): the role of spin selection rules. *Physical Review Letters*, **2005**, 94, 036104	7.4	234
75	Binding energies, molecular structures, and vibrational frequencies of transition metal carbonyls using density functional theory with gradient corrections. *Journal of Chemical Physics*, **1994**, 100, 5785-5791	3.9	229
74	Oxygen adsorption and stability of surface oxides on Cu(111): A first-principles investigation. *Physical Review B*, **2006**, 73,	3.3	216
73	Spin density in a nitronyl nitroxide free radical. Polarized neutron diffraction investigation and ab initio calculations. *Journal of the American Chemical Society*, **1994**, 116, 2019-2027	16.4	207
72	Water adsorption on the stoichiometric and reduced CeO2(111) surface: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2009**, 11, 9188-99	3.6	198
71	Gas-phase-dependent properties of SnO2 (110), (100), and (101) single-crystal surfaces: Structure, composition, and electronic properties. *Physical Review B*, **2005**, 72,	3.3	185
70	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. *Journal of Chemical Physics*, **2009**, 131, 104701	3.9	129
69	Superhard nitride-based nanocomposites: role of interfaces and effect of impurities. *Physical Review Letters*, **2006**, 97, 086102	7.4	114
68	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of Cu2O. *Physical Review B*, **2009**, 79,	3.3	96
67	Evidence for Transmission of Ferromagnetic Interactions through Hydrogen Bonds in Alkyne-Substituted Nitroxide Radicals: Magnetostructural Correlations and Polarized Neutron Diffraction Studies. *Journal of the American Chemical Society*, **2000**, 122, 1298-1309	16.4	96
66	Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles. *Physical Review B*, **2008**, 77,	3.3	77
65	Nonadiabatic potential-energy surfaces by constrained density-functional theory. *Physical Review B*, **2007**, 75,	3.3	75
64	Photogeneration of two metastable NO linkage isomers with high populations of up to 76% in trans-[RuCl(py)4(NO)][PF6]2.1/2H2O. *Physical Chemistry Chemical Physics*, **2007**, 9, 3717-24	3.6	72

63	Structure and properties of TiN(111)/SixNy/TiN(111) interfaces in superhard nanocomposites: First-principles investigations. *Physical Review B*, **2006**, 74,	3.3	66
62	Spin Density Maps for the Ferrimagnetic Chain Compound MnCu(pba)(H2O)3·2H2O (pba = 1,2-Propylenebis(oxamato)): Polarized Neutron Diffraction and Theoretical Studies. *Journal of the American Chemical Society*, **1997**, 119, 3500-3506	16.4	62
61	Questioning the existence of a unique ground-state structure for Si clusters. *Physical Review B*, **2007**, 75,	3.3	62
60	Bridging Hydroxyl Groups in Faujasite: Periodic vs Cluster Density Functional Calculations. *Journal of Physical Chemistry A*, **1999**, 103, 3772-3777	2.8	62
59	Surface structure of Sn-doped In2O3(111) thin films by STM. *New Journal of Physics*, **2008**, 10, 125030	2.9	60
58	Long-lived light-induced metastable states in trans-[Ru(NH3)4(H2O)NOCl3 x H2O and related compounds. *Physical Chemistry Chemical Physics*, **2005**, 7, 1164-70	3.6	60
57	[Ru(py)4Cl(NO)](PF6)2.0.5H2O: a model system for structural determination and ab initio calculations of photo-induced linkage NO isomers. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 612-23		58
56	Surface oxides of the oxygen/copper system: Precursors to the bulk oxide phase?. *Surface Science*, **2007**, 601, 5809-5813	1.8	57
55	Spin-Density Maps for an Oxamido-Bridged Mn(II)Cu(II) Binuclear Compound. Polarized Neutron Diffraction and Theoretical Studies. *Journal of the American Chemical Society*, **1996**, 118, 11822-11830	16.4	56
54	The effect of grid quality and weight derivatives in density functional calculations. *Journal of Chemical Physics*, **1994**, 101, 8894-8902	3.9	50
53	Spectroscopic and theoretical studies of metal cluster complexes. Part 2. X.alpha. calculations and spectroscopic studies of triruthenium and triosmium dodecacarbonyls. *Inorganic Chemistry*, **1982**, 21, 2247-2253	5.1	49
52	High order integration schemes on the unit sphere. *Journal of Computational Chemistry*, **1996**, 17, 1152-1155	3.5	46
51	Light harvesting with multiwall carbon nanotube/silicon heterojunctions. *Nanotechnology*, **2011**, 22, 115701	3.4	43
50	Role of oxygen in TiN(111)/SixNy/TiN(111) interfaces: Implications for superhard nanocrystalline nc-TiN/Si3N4 nanocomposites. *Physical Review B*, **2006**, 74,	3.3	43
49	Quantum chemical analysis of electronic structure and n- and p-type charge transport in perfluoroarene-modified oligothiophene semiconductors. *Journal of Physical Chemistry B*, **2006**, 110, 24361-70	3.4	43
48	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). *Physical Review B*, **2008**, 78,	3.3	42
47	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. *Surface Science*, **2007**, 601, 4775-4785	1.8	38
46	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. *Physical Review B*, **2008**, 77,	3.3	36

45	Mn-doped CuGaS2 chalcopyrites: An ab initio study of ferromagnetic semiconductors. *Physical Review B*, **2002**, 66,	3.3	36
44	Dissociation of Water on Anatase TiO2 Nanoparticles: the Role of Undercoordinated Ti Atoms at Edges. *Journal of Physical Chemistry C*, **2009**, 113, 15862-15867	3.8	33
43	Tunable conductivity and conduction mechanism in an ultraviolet light activated electronic conductor. *Journal of Applied Physics*, **2005**, 97, 103713	2.5	33
42	Electronic structure of endohedral fullerenes An@C28 (An=Th Md). *Computational and Theoretical Chemistry*, **2012**, 985, 46-52	2	32
41	Electronic structure and oxygen vacancies in PdO and ZnO: validation of DFT models. *Physical Chemistry Chemical Physics*, **2011**, 13, 15947-54	3.6	32
40	Generation of one light-induced metastable nitrosyl linkage isomer in [Pt(NH3)4Cl(NO)]Cl2 in the red spectral range. *Physical Chemistry Chemical Physics*, **2007**, 9, 5149-57	3.6	32
39	Massive thermostatting in isothermal density functional molecular dynamics simulations. *Journal of Chemical Physics*, **2003**, 119, 2481-2487	3.9	31
38	Reaction intermediates of methanol synthesis and the water gas-shift reaction on the ZnO(0001) surface. *Surface Science*, **2010**, 604, 1742-1751	1.8	28
37	Reversible photoswitching between nitrito-N and nitrito-O isomers in trans-[Ru(py)(4)(NO(2))(2)]. *Physical Chemistry Chemical Physics*, **2010**, 12, 6171-8	3.6	27
36	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. *Nanoscale*, **2012**, 4, 5183-8	7.7	25
35	Gap opening in the surface electronic structure of graphite induced by adsorption of alkali atoms: Photoemission experiments and density functional calculations. *Physical Review B*, **2005**, 71,	3.3	24
34	Why does bromine square palladium off? An ab initio study of brominated palladium and its nanomorphology. *Physical Chemistry Chemical Physics*, **2014**, 16, 18570-7	3.6	22
33	Combined Ab Initio Total Energy Density Functional Calculations and Scanning Tunneling Microscopy Experiments of the SiC(001) c(4x2) Surface. *Materials Science Forum*, **1998**, 264-268, 379-382	0.4	21
32	Photogeneration of nitrosyl linkage isomers in octahedrally coordinated platinum complexes in the red spectral range. *Inorganic Chemistry*, **2009**, 48, 11399-406	5.1	20
31	Photogeneration of metastable side-on N2 linkage isomers in [Ru(NH3)5N2]Cl2, [Ru(NH3)5N2]Br2 and [Os(NH3)5N2]Cl2. *Physical Chemistry Chemical Physics*, **2008**, 10, 5531-8	3.6	20
30	Observation of a Fano Resonance in Photoemission. *Physical Review Letters*, **1999**, 82, 2971-2974	7.4	19
29	Electronic structure of predicted endohedral fullerenes An@C40 (An=Th Md). *Computational and Theoretical Chemistry*, **2013**, 1013, 70-77	2	18
28	A first-principles study of ultrathin nanofilms of MgO-supported TiN. *Physical Chemistry Chemical Physics*, **2012**, 14, 2462-7	3.6	18

27	Spin density in a triazole-nitronyl-nitroxide radical presenting linear ferromagnetic interactions: role of hydrogen bonding. *Chemical Physics*, **1999**, 250, 23-34	2.3	18
26	Interaction between zigzag single-wall carbon nanotubes and polymers: a density-functional study. *Journal of Chemical Physics*, **2005**, 122, 214710	3.9	17
25	DFT study of structural and vibrational properties of guanidinium derivatives. *Computational and Theoretical Chemistry*, **2009**, 907, 16-21		14
24	CHx adsorption (x = 1⁄4) and thermodynamic stability on the CeO2(111) surface: a first-principles investigation. *RSC Advances*, **2014**, 4, 12245	3.7	13
23	Quantum confinement effects in gallium nitride nanostructures: ab initio investigations. *Nanotechnology*, **2009**, 20, 425401	3.4	13
22	Guanidinium Formate Decomposition on the (101) TiO2-Anatase Surface: Combined Minimum Energy Reaction Pathway Calculations and Temperature-Programmed Decomposition Experiments *Journal of Physical Chemistry C*, **2011**, 115, 1195-1203	3.8	12
21	A DFT Study of the Energetical and Structural Landscape of the Tetrahedral to Square-Planar Conversion of Tetrahalide Complexes of Copper(II) *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2010**, 636, 1740-1750	1.3	12
20	The Creutz-Taube complex revisited: DFT study of the infrared frequencies. *Inorganic Chemistry*, **2008**, 47, 11269-77	5.1	8
19	Brillouin zone folding and Fano resonances in commensurate rare gas monolayers observed in photoemission. *Surface Science*, **2000**, 454-456, 483-488	1.8	7
18	Early transition metal dopants in cuprous oxide: To spin or not to spin. *Current Applied Physics*, **2013** , 13, 1707-1712	2.6	6
17	[Ru(py)4Cl(NO)](PF6)2 0.5H2O: a model system for structural determination and ab initio calculations of photo-induced linkage NO isomers. Erratum. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 787-787		6
16	DFT study of crystalline nitrosyl compounds. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2008**, 223, 329-333	1	6
15	Molecular adsorption and methanol synthesis on the oxidized Cu/ZnO(0001) surface. *Surface Science*, **2015**, 641, 97-104	1.8	5
14	Enhancing Hydrophilicity of Anatase TiO2 Surfaces by Deposition of Alkaline Earths: The Case of Ca. *Journal of Physical Chemistry C*, **2013**, 117, 26013-26020	3.8	5
13	Aluminium adsorption on Ir(1 1 1) at a quarter monolayer coverage: A first-principles study. *Applied Surface Science*, **2008**, 254, 7655-7658	6.7	3
12	Density-functional calculations of Esterel twinning in quartz. *Physical Review B*, **2007**, 76,	3.3	3
11	Crystal structures and electronic properties of haloform-intercalated C60. *Physical Review B*, **2002**, 66,	3.3	3
10	Evolution of the Electronic and Geometric Structure of Size Selected Pt and Pd Clusters on Ag(110) Observed by Photoemission. *Materials Science Forum*, **1996**, 232, 51-66	0.4	3

9	Density functional calculations of polysynthetic Brazil twinning in □quartz. *Acta Crystallographica Section A: Foundations and Advances*, **2012**, 68, 359-65		2
8	Fast full-field modulation transfer function analysis for photographic lens quality assessment. *Applied Optics*, **2021**, 60, 2197-2206	1.7	2
7	Long-Lived Light-Induced Metastable States in trans-[Ru(NH3)4(H2O)NO] Cl3□H2O and Related Compounds.. *ChemInform*, **2005**, 36, no		1
6	Plutonium complexes in water: new approach to ab initio modeling. *Radiochimica Acta*, **2021**, 109, 327-342	1.9	1
5	Comparison of experimental and theoretical results for the structure and elastic properties of moganite. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2017**, 232, 279-286	1	
4	Fano spectroscopy of impurities and clusters on solid surfaces. *Journal of Electron Spectroscopy and Related Phenomena*, **2002**, 124, 195-210	1.7	
3	Wetting of Paracetamol Surfaces Studied by DMol3-COSMO Calculations **2011**, 37-46		
2	First-principles study on the plutonium ions interaction with diamide molecules in acid solutions. *International Journal of Quantum Chemistry*, **2021**, 121, e26681	2.1	
1	Density functional theory calculations of merohedric twinning in KLiSO4. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2019**, 234, 211-217	1	