Philippe D'Arco

List of Publications by Year
in descending order

18	1,550	933447 10	839539 18
papers	citations	h-index	g-index

18	18	18	2370
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	C<scp>RYSTAL14</scp>: A program for the ab initio investigation of crystalline solids. International Journal of Quantum Chemistry, 2014, 114, 1287-1317.	2.0	1,151
2	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
3	On the use of symmetry in the ab initio quantum mechanical simulation of nanotubes and related materials. Journal of Computational Chemistry, 2010, 31, 855-862.	3.3	48
4	Structure and energetics of imogolite: a quantum mechanical ab initio study with B3LYP hybrid functional. Journal of Materials Chemistry, 2010, 20, 10417.	6.7	41
5	On the use of symmetry in configurational analysis for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 105401.	1.8	34
6	Single-layered chrysotile nanotubes: A quantum mechanical ab initio simulation. Journal of Chemical Physics, 2009, 131, 204701.	3.0	26
7	Symmetry and random sampling of symmetry independent configurations for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 355401.	1.8	24
8	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	2.8	17
9	Hydrogrossular, Ca₃Al₂(SiO₄)_{3â€“x}(H₄O₄)_x: An ab initio investigation of its structural and energetic properties. American Mineralogist, 2015, 100, 2637-2649.	1.9	16
10	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
11	The Infrared spectrum of very large (periodic) systems: global versus fragment strategiesâ€”the case of three defects in diamond. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	10
12	Strategies for the optimization of the structure of crystalline compounds. Journal of Computational Chemistry, 2022, 43, 184-196.	3.3	9
13	Substitutional carbon defects in silicon: A quantum mechanical characterization through the infrared and Raman spectra. Journal of Computational Chemistry, 2020, 41, 1638-1644.	3.3	8
14	The ferromagnetic and anti-ferromagnetic phases (cubic, tetragonal, orthorhombic) of KMnF₃. A quantum mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 26780-26792.	2.8	7
15	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	2.2	3
16	The superexchange mechanism in crystalline compounds. The case of KMF₃ (M = Mn, Fe, Co,) Tj ETQq0 0 0 rgBT /Overlock	1.8	3
17	On the use of the symmetry-adapted Monte Carlo for an effective sampling of large configuration spaces. The test cases of calcite structured carbonates and melilites. Computational Materials Science, 2017, 126, 217-227.	3.0	2
18	Interstitial carbon defects in silicon. A quantum mechanical characterization through the infrared and Raman spectra. Journal of Computational Chemistry, 2021, 42, 806-817.	3.3	2