

# Philippe D'Arco

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/563823/publications.pdf>

Version: 2024-02-01

18  
papers

1,550  
citations

932766

10  
h-index

839053

18  
g-index

18  
all docs

18  
docs citations

18  
times ranked

2370  
citing authors

#	ARTICLE	IF	CITATIONS
1	C<sc>RYSTAL14</sc>: A program for the <i>ab initio</i> investigation of crystalline solids. International Journal of Quantum Chemistry, 2014, 114, 1287-1317.	1.0	1,151
2	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	1.2	133
3	On the use of symmetry in the <i>ab initio</i> quantum mechanical simulation of nanotubes and related materials. Journal of Computational Chemistry, 2010, 31, 855-862.	1.5	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.	0.7	34
6	Single-layered chrysotile nanotubes: A quantum mechanical <i>ab initio</i> simulation. Journal of Chemical Physics, 2009, 131, 204701.	1.2	26
7	Symmetry and random sampling of symmetry independent configurations for the simulation of disordered solids. Journal of Physics Condensed Matter, 2013, 25, 355401.	0.7	24
8	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	1.3	17
9	Hydrogrossular, Ca<sub>3</sub>Al<sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>(H<sub>4</sub>O<sub>4</sub>)<sub>x</sub>: An ab initio investigation of its structural and energetic properties. American Mineralogist, 2015, 100, 2637-2649.	0.9	16
10	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	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.	0.5	10
12	Strategies for the optimization of the structure of crystalline compounds. Journal of Computational Chemistry, 2022, 43, 184-196.	1.5	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.	1.5	8
14	The ferromagnetic and anti-ferromagnetic phases (cubic, tetragonal, orthorhombic) of KMnF<sub>3</sub>. A quantum mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 26780-26792.	1.3	7
15	From anisotropy of dielectric tensors to birefringence: a quantum mechanics approach. Rendiconti Lincei, 2020, 31, 835-851.	1.0	3
16	The superexchange mechanism in crystalline compounds. The case of KMF<sub>3</sub> (M = Mn, Fe, Co,) Tj ETQq0 0 0 rgBT <sub>3</sub> /Overlock	0.7	0
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.	1.4	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.	1.5	2