Francesco Silvio Gentile

List of Publications by Year
in descending order

40 papers	572 citations	687363 13 h-index	642732 23 g-index
40 all docs	40 docs citations	40 times ranked	434 citing authors

#	Article	IF	Citations
1	The NV0 defects in diamond: A quantum mechanical characterization through its vibrational and Electron Paramagnetic Resonance spectroscopies. Journal of Physics and Chemistry of Solids, 2022, 160, 110304.	4.0	3
2	Strategies for the optimization of the structure of crystalline compounds. Journal of Computational Chemistry, 2022, 43, 184-196.	3.3	9
3	Benzodifuran-based fluorescent brighteners: A novel platform for plant cell wall imaging. Dyes and Pigments, 2022, 199, 110071.	3.7	3
4	The calculated energies and charge and spin distributions of the excited GR1 state in diamond. Journal of Chemical Physics, 2022, 156, 044708.	3.0	7
5	Structural feature of thermo-induced fluorochromism in a 1D zinc coordination polymer. A cross-analysis by PL and FTIR spectroscopy, and DFT formalism. Dyes and Pigments, 2022, 202, 110247.	3.7	5
6	Thermo-Induced Fluorochromism in Two AIE Zinc Complexes: A Deep Insight into the Structure-Property Relationship. Molecules, 2022, 27, 2551.	3.8	3
7	Colorimetric recognition of multiple first-row transition metals: A single water-soluble chemosensor in acidic and basic conditions. Dyes and Pigments, 2021, 184, 108832.	3.7	15
8	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
9	Oxygen and vacancy defects in silicon. A quantum mechanical characterization through the IR and Raman spectra. Journal of Chemical Physics, 2021, 154, 174707.	3.0	4
10	Fluorescence pH-dependent sensing of zinc (II) and chromium (III) cations by a tripodal ligand and exploration of emission response in solution and in the solid state. Dyes and Pigments, 2021, 193, 109567.	3.7	0
11	Vibrational Analysis of Paraelectricâ€“Ferroelectric Transition of LiNbO3: An Ab-Initio Quantum Mechanical Treatment. Symmetry, 2021, 13, 1650.	2.2	2
12	The NVâ¯â‹¯N+ charged pair in diamond: a quantum-mechanical investigation. Physical Chemistry Chemical Physics, 2021, 23, 18724-18733.	2.8	2
13	The effect of charge and spin state on the Infrared spectra and hyperfine coupling constants of point defects in Silicon. Physica B: Condensed Matter, 2021, 626, 413499.	2.7	0
14	Characterization of the negatively charged NV defect through the spin density distribution and the hyperfine coupling constants. Journal of Physics and Chemistry of Solids, 2021, , 110506.	4.0	0
15	A Novel L-Shaped Fluorescent Probe for AIE Sensing of Zinc (II) Ion by a DR/NIR Response. Molecules, 2021, 26, 7347.	3.8	6
16	The VN2 negatively charged defect in diamond. A quantum mechanical investigation of the EPR response. Carbon, 2020, 159, 443-450.	10.3	17
17	Hierarchy of Intermolecular Interactions and Selective Topochemical Reactivity in Different Polymorphs of Fused-Ring Heteroaromatics. Crystal Growth and Design, 2020, 20, 1229-1236.	3.0	13
18	The VN defect in diamond: A quantum mechanical simulation of the vibrational spectra and EPR properties. Carbon, 2020, 170, 600-605.	10.3	5

#	Article	IF	Citations
19	Interstitial defects in diamond: A quantum mechanical simulation of their EPR constants and vibrational spectra. Journal of Chemical Physics, 2020, 153, 024119.	3.0	6
20	Microscopic Characterization of Oxygen Defects in Diamond as Models for N3 and OK1 Defects: A Comparison of Calculated and Experimental Electron Paramagnetic Resonance Data. Journal of Physical Chemistry A, 2020, 124, 8263-8272.	2.5	2
21	Predicted strong spin-phonon interactions in Li-doped diamond. Physical Chemistry Chemical Physics, 2020, 22, 20612-20617.	2.8	5
22	Metal defects in HKUST-1 MOF revealed by vibrational spectroscopy: a combined quantum mechanical and experimental study. Journal of Materials Chemistry A, 2020, 8, 10796-10812.	10.3	43
23	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	3.0	133
24	N₂ positively charged defects in diamond. A quantum mechanical investigation of the structural, electronic, EPR and vibrational properties. Journal of Materials Chemistry C, 2020, 8, 5239-5247.	5.5	10
25	An all-electron study of the low-lying excited states and optical constants of Al₂O₃ in the range 5â€“80 eV. Journal of Physics Condensed Matter, 2020, 32, 085901.	1.8	8
26	The spectroscopic characterization of interstitial oxygen in bulk silicon: A quantum mechanical simulation. Journal of Chemical Physics, 2020, 152, 054502.	3.0	5
27	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
28	Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Materials Today Communications, 2019, 21, 100616.	1.9	9
29	Nitrogen substitutional defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Physical Chemistry Chemical Physics, 2019, 21, 20939-20950.	2.8	19
30	On the Models for the Investigation of Charged Defects in Solids: The Case of the VN^{â€“} Defect in Diamond. Journal of Physical Chemistry A, 2019, 123, 4806-4815.	2.5	4
31	The characterization of the VN H defects in diamond through the infrared vibrational spectrum. A quantum mechanical investigation. Carbon, 2018, 132, 210-219.	10.3	20
32	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. Physical Chemistry Chemical Physics, 2018, 20, 11930-11940.	2.8	17
33	Substitutional nitrogen in diamond: A quantum mechanical investigation of the electronic and spectroscopic properties. Carbon, 2018, 134, 354-365.	10.3	42
34	Strong Metalâ€“Support Interactions of TiNâ€“ and TiO₂â€“Nickel Nanocomposite Catalysts. Journal of Physical Chemistry C, 2018, 122, 339-348.	3.1	22
35	Characterization of the B-Center Defect in Diamond through the Vibrational Spectrum: A Quantum-Mechanical Approach. Journal of Physical Chemistry A, 2018, 122, 594-600.	2.5	23
36	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16

#	Article	IF	Citations
37	The VN₃H defect in diamond: a quantum-mechanical characterization. Physical Chemistry Chemical Physics, 2017, 19, 22221-22229.	2.8	20
38	Hindered Brownian diffusion in a square-shaped geometry. Journal of Colloid and Interface Science, 2015, 447, 25-32.	9.4	9
39	Experimental evidence of stable water nanostructures in extremely dilute solutions, at standard pressure and temperature. Homeopathy, 2014, 103, 44-50.	1.0	53
40	Effect of chalcogen bonding on the packing and coordination geometry in hybrid organicâ€“inorganic Cu(<scp>ii</scp>) networks. CrystEngComm, 0, , .	2.6	2