Margherita Marsili

List of Publications by Year
in descending order

38 papers	5,481 citations	471509 17 h-index	315739 38 g-index
39 all docs	39 docs citations	39 times ranked	8171 citing authors

#	Article	IF	Citations
1	Electronic Dynamics of a Molecular System Coupled to a Plasmonic Nanoparticle Combining the Polarizable Continuum Model and Many-Body Perturbation Theory. Journal of Physical Chemistry C, 2022, 126, 8768-8776.	3.1	3
2	Spinorial formulation of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m -BSE equations and spin properties of excitons in two-dimensional transition metal dichalcogenides. Physical Review B, 2021, 103, .	3.2	16
3	Study of the Rate-Determining Step of Rh Catalyzed CO2 Reduction: Insight on the Hydrogen Assisted Molecular Dissociation. Catalysts, 2021, 11, 538.	3.5	6
4	Optical detection of the susceptibility tensor in two-dimensional crystals. Communications Physics, 2021, 4, .	5.3	26
5	Time-Resolved Excited-State Analysis of Molecular Electron Dynamics by TDDFT and Betheâ€“Salpeter Equation Formalisms. Journal of Chemical Theory and Computation, 2021, 17, 6314-6329.	5.3	8
6	Hybrid theoretical models for molecular nanoplasmonics. Journal of Chemical Physics, 2020, 153, 200901.	3.0	27
7	Surface susceptibility and conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></m monolayers: A first-principles and ellipsometry characterization. Physical Review B, 2020, 101, .	3.2	28
8	Koopmans Meets Betheâ€“Salpeter: Excitonic Optical Spectra without GW. Journal of Chemical Theory and Computation, 2019, 15, 3710-3720.	5.3	20
9	Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902.	1.8	269
10	Large-scale <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m -BSE calculations with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>N</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:m scaling: Excitonic effects in dye-sensitized solar cells. Physical Review B, 2017, 95, .	3.2	34
11	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
12	Photo-Induced Bandgap Renormalization Governs the Ultrafast Response of Single-Layer MoS₂. ACS Nano, 2016, 10, 1182-1188.	14.6	272
13	Excitons in two-dimensional sheets with honeycomb symmetry. Physica Status Solidi (B): Basic Research, 2015, 252, 72-77.	1.5	23
14	Alignment of energy levels in dye/semiconductor interfaces by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m Effects due to coadsorption of solvent molecules. Physical Review B, 2014, 90, .	3.2	18
15	Solid state effects on the electronic structure of H₂OEP. Physical Chemistry Chemical Physics, 2014, 16, 27104-27111.	2.8	6
16	Thermal and electrical characterization of catastrophic degradation of silicon solar cells submitted to reverse current stress. , 2013, , .		3
17	Ab Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects. Journal of Physical Chemistry C, 2013, 117, 14229-14234.	3.1	12
18	Method for the fast evaluation of Fock exchange for nonlocalized wave functions. Physical Review B, 2013, 87, .	3.2	8

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19	Side-dependent electron escape from graphene- and graphane-like SiC layers. Applied Physics Letters, 2012, 100, .	3.3	39
20	Excited state properties of formamide in water solution: An ab initio study. Journal of Chemical Physics, 2012, 137, 164317.	3.0	2
21	Technological and economic assessment of two-steps printing processes in a mc-Si solar cells production environment. Energy Procedia, 2012, 21, 24-31.	1.8	5
22	Strong excitons in novel two-dimensional crystals: Silicane and germanane. Europhysics Letters, 2012, 98, 37004.	2.0	112
23	Defect induced modification of the surface gap and optical properties of C(111)2â€‰Ã—â€‰1 surface. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 669-674.	1.8	4
24	Contribution of steps to optical properties of vicinal diamond (100):H surfaces. Physical Review B, 2011, 83, .	3.2	7
25	Local-field effects in silicon nanoclusters. Physical Review B, 2011, 84, .	3.2	17
26	Electronic and optical properties of Si and Ge nanocrystals: An ab initio study. Superlattices and Microstructures, 2010, 47, 178-181.	3.1	1
27	Electronic and optical properties of group IV twoâ€dimensional materials. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 291-299.	1.8	21
28	Localâ€fields and disorder effects in freeâ€standing and embedded Si nanocrystallites. Physica Status Solidi (B): Basic Research, 2010, 247, 2113-2117.	1.5	9
29	The fascinating physics of carbon surfaces: first-principles study of hydrogen on C(0â€‰0â€‰1), C(1â€‰1â€‰1) and graphene. Journal Physics D: Applied Physics, 2010, 43, 374016.	2.8	16
30	Electronic and optical properties of acetylene and ethylene on Si(001). Superlattices and Microstructures, 2009, 46, 240-245.	3.1	3
31	Adsorption of small hydrocarbon molecules on Si surfaces: Ethylene on Si(001). Physical Review B, 2008, 77, .	3.2	30
32	Tight-binding calculations of quasiparticle wave functions forC(111)2Ã—1. Physical Review B, 2008, 78, .	3.2	13
33	First-Principles Study of Silicon Nanocrystals: Structural and Electronic Properties, Absorption, Emission, and Doping. Journal of Nanoscience and Nanotechnology, 2008, 8, 479-492.	0.9	25
34	Efficientab initiocalculations of bound and continuum excitons in the absorption spectra of semiconductors and insulators. Physical Review B, 2007, 76, .	3.2	47
35	Many body effects in the electronic and optical properties of the (111) surface of diamond. Surface Science, 2007, 601, 4097-4101.	1.9	4
36	Geometry and electronic band structure of surfaces: the case of Ge(111):Sn and C(111). Applied Physics A: Materials Science and Processing, 2006, 85, 361-369.	2.3	10

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37	Electronic excitations in solids: Density functional and Green's function theory. Physica Status Solidi (B): Basic Research, 2005, 242, 2737-2750.	1.5	11
38	Electronic structure of theC(111)surface: Solution by self-consistent many-body calculations. Physical Review B, 2005, 72, .	3.2	26