

# Roberta Poloni

## List of Publications by Year in descending order

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32  
papers

2,476  
citations

430754

18  
h-index

414303

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g-index

37  
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37  
docs citations

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times ranked

3912  
citing authors

#	ARTICLE	IF	CITATIONS
1	Probing the $SO_2$ Adsorption Mechanism in Hofmann Clathrates via Inelastic Neutron Scattering and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8090-8099.	1.5	7
2	Bethe-Salpeter Study of the Optical Absorption of <i>trans</i> and <i>cis</i> Azobenzene-Functionalized Metal-Organic Frameworks Using Molecular and Periodic Models. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7401-7412.	1.5	9
3	Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes via the Hubbard $U$ -Corrected Density. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2807-2816.	2.3	22
4	Strongly Bound Excitons in Metal-Organic Framework MOF-5: A Many-Body Perturbation Theory Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4045-4051.	2.1	15
5	Electric field-induced oxygen vacancies in $YBa_2Cu_3O_7$ . <i>Journal of Chemical Physics</i> , 2021, 154, 224703.	1.2	2
6	Tunable Proton Conductivity and Color in a Nonporous Coordination Polymer via Lattice Accommodation to Small Molecules. <i>Advanced Science</i> , 2021, 8, e2102619.	5.6	7
7	Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density-Functional Theory and the Linear-Response Hubbard $U$ Correction. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6755-6762.	2.3	23
8	Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metal-Organic Frameworks for Highly Sensitive $NO_2$ Sensors. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3362-3368.	2.1	50
9	Accurate Prediction of the $S_1$ Excitation Energy in Solvated Azobenzene Derivatives via Embedded Orbital-Tuned Bethe-Salpeter Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2021-2027.	2.3	10
10	A switchable iron-based coordination polymer toward reversible acetonitrile electro-optical readout. <i>Chemical Science</i> , 2019, 10, 6612-6616.	3.7	26
11	Probing the electric field-induced doping mechanism in $YBa_2Cu_3O_7$ using computed Cu K-edge x-ray absorption spectra. <i>Journal of Chemical Physics</i> , 2018, 149, 234706.	1.2	8
12	Role of Impurities in the Kinetic Persistence of Amorphous Calcium Carbonate: A Nanoscopic Dynamics View. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16983-16991.	1.5	35
13	Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2018, 24, 15167-15172.	1.7	33
14	<i>In operando</i> evidence of deoxygenation in ionic liquid gating of $YBa_2Cu_3O_{7-x}$ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 215-220.	3.3	51
15	Long-range magnetic order in the porous metal-organic framework $Ni(\text{pyrazine})[Pt(CN)_4]$ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29084-29091.	1.3	3
16	Wetting layer of copper on the tantalum (001) surface. <i>Physical Review B</i> , 2016, 94, .	1.1	6
17	Thermodynamics of gas adsorption in MOFs using <i>Ab Initio</i> calculations. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 569-572.	1.0	9
18	Probing gas adsorption in MOFs using an efficient <i>ab initio</i> wisdom insertion Monte Carlo method. <i>Journal of Computational Chemistry</i> , 2016, 37, 2808-2815.	1.5	8

#	ARTICLE	IF	CITATIONS
19	Cooperative insertion of CO <sub>2</sub> in diamine-appended metal-organic frameworks. <i>Nature</i> , 2015, 519, 303-308.	13.7	1,026
20	Probing the mechanism of CO <sub>2</sub> capture in diamine-appended metal-organic frameworks using measured and simulated X-ray spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21448-21457.	1.3	43
21	Predicting low-k zeolite materials. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2298-2300.	2.7	10
22	Understanding Trends in CO <sub>2</sub> Adsorption in Metal-Organic Frameworks with Open-Metal Sites. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 861-865.	2.1	139
23	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2013, 135, 7402-7405.	6.6	208
24	Probing Adsorption Interactions in Metal-Organic Frameworks using X-ray Spectroscopy. <i>Journal of the American Chemical Society</i> , 2013, 135, 18183-18190.	6.6	56
25	CO <sub>2</sub> Capture by Metal-Organic Frameworks with van der Waals Density Functionals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4957-4964.	1.1	92
26	Ligand-Assisted Enhancement of CO <sub>2</sub> Capture in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2012, 134, 6714-6719.	6.6	95
27	Ab initio carbon capture in open-site metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 810-816.	6.6	310
28	An efficient computational method for use in structural studies of crystals with substitutional disorder. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 415401.	0.7	9
29	Concerning the Possibility of Hidden One-Dimensional Fermi Surfaces for the K <sub>0.25</sub> WO <sub>3</sub> Hexagonal Bronze. <i>Inorganic Chemistry</i> , 2009, 48, 11492-11494.	1.9	3
30	A diamond anvil cell with resistive heating for high pressure and high temperature x-ray diffraction and absorption studies. <i>Review of Scientific Instruments</i> , 2008, 79, 085103.	0.6	36
31	Optimization of Paris-Edinburgh press cell assemblies for <i>in situ</i> monochromatic X-ray diffraction and X-ray absorption. <i>High Pressure Research</i> , 2007, 27, 223-233.	0.4	48
32	Structure of eutectic Fe-FeS melts to pressures up to 17 GPa: Implications for planetary cores. <i>Earth and Planetary Science Letters</i> , 2007, 263, 128-139.	1.8	77