# Roberta Poloni

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4971229/publications.pdf

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|---|---|---|---|
| 32 papers | 2,476 citations | 430754 18 h-index | 414303 32 g-index |
| 37 all docs | 37 docs citations | 37 times ranked | 3912 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308. | 13.7 | 1,026 |
| 2 | Ab initio carbon capture in open-site metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 810-816. | 6.6 | 310 |
| 3 | The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 7402-7405. | 6.6 | 208 |
| 4 | Understanding Trends in CO<sub>2</sub> Adsorption in Metalâ€“Organic Frameworks with Open-Metal Sites. Journal of Physical Chemistry Letters, 2014, 5, 861-865. | 2.1 | 139 |
| 5 | Ligand-Assisted Enhancement of CO<sub>2</sub> Capture in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 6714-6719. | 6.6 | 95 |
| 6 | CO2 Capture by Metalâ€“Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964. | 1.1 | 92 |
| 7 | Structure of eutectic Feâ€“FeS melts to pressures up to 17ÂGPa: Implications for planetary cores. Earth and Planetary Science Letters, 2007, 263, 128-139. | 1.8 | 77 |
| 8 | Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190. | 6.6 | 56 |
| 9 | In operando evidence of deoxygenation in ionic liquid gating of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-X</sub>. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 215-220. | 3.3 | 51 |
| 10 | Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metalâ€“Organic Frameworks for Highly Sensitive NO<sub>2</sub> Sensors. Journal of Physical Chemistry Letters, 2020, 11, 3362-3368. | 2.1 | 50 |
| 11 | Optimization of Parisâ€“Edinburgh press cell assemblies forin situmonochromatic X-ray diffraction and X-ray absorption. High Pressure Research, 2007, 27, 223-233. | 0.4 | 48 |
| 12 | Probing the mechanism of CO<sub>2</sub> capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457. | 1.3 | 43 |
| 13 | A diamond anvil cell with resistive heating for high pressure and high temperature x-ray diffraction and absorption studies. Review of Scientific Instruments, 2008, 79, 085103. | 0.6 | 36 |
| 14 | Role of Impurities in the Kinetic Persistence of Amorphous Calcium Carbonate: A Nanoscopic Dynamics View. Journal of Physical Chemistry C, 2018, 122, 16983-16991. | 1.5 | 35 |
| 15 | Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2018, 24, 15167-15172. | 1.7 | 33 |
| 16 | A switchable iron-based coordination polymer toward reversible acetonitrile electro-optical readout. Chemical Science, 2019, 10, 6612-6616. | 3.7 | 26 |
| 17 | Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density-Functional Theory and the Linear-Response Hubbard U Correction. Journal of Chemical Theory and Computation, 2020, 16, 6755-6762. | 2.3 | 23 |
| 18 | Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes via the Hubbard U-Corrected Density. Journal of Chemical Theory and Computation, 2021, 17, 2807-2816. | 2.3 | 22 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Strongly Bound Excitons in Metalâ€“Organic Framework MOF-5: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry Letters, 2021, 12, 4045-4051. | 2.1 | 15 |
| 20 | Predicting low-k zeolite materials. Journal of Materials Chemistry C, 2014, 2, 2298-2300. | 2.7 | 10 |
| 21 | Accurate Prediction of the S<sub>1</sub> Excitation Energy in Solvated Azobenzene Derivatives via Embedded Orbital-Tuned Bethe-Salpeter Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2021-2027. | 2.3 | 10 |
| 22 | An efficient computational method for use in structural studies of crystals with substitutional disorder. Journal of Physics Condensed Matter, 2010, 22, 415401. | 0.7 | 9 |
| 23 | Thermodynamics of gas adsorption in <scp>MOF</scp>s using Ab Initio calculations. International Journal of Quantum Chemistry, 2016, 116, 569-572. | 1.0 | 9 |
| 24 | Betheâ€“Salpeter Study of the Optical Absorption of trans and cis Azobenzene-Functionalized Metalâ€“Organic Frameworks Using Molecular and Periodic Models. Journal of Physical Chemistry C, 2021, 125, 7401-7412. | 1.5 | 9 |
| 25 | Probing gas adsorption in MOFs using an efficient ab initio widom insertion Monte Carlo method. Journal of Computational Chemistry, 2016, 37, 2808-2815. | 1.5 | 8 |
| 26 | Probing the electric field-induced doping mechanism in YBa2Cu3O7 using computed Cu K-edge x-ray absorption spectra. Journal of Chemical Physics, 2018, 149, 234706. | 1.2 | 8 |
| 27 | Tunable Proton Conductivity and Color in a Nonporous Coordination Polymer via Lattice Accommodation to Small Molecules. Advanced Science, 2021, 8, e2102619. | 5.6 | 7 |
| 28 | Probing the SO<sub>2</sub>Adsorption Mechanism in Hofmann Clathrates via Inelastic Neutron Scattering and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2022, 126, 8090-8099. | 1.5 | 7 |
| 29 | Wetting layer of copper on the tantalum (001) surface. Physical Review B, 2016, 94, . | 1.1 | 6 |
| 30 | Concerning the Possibility of Hidden One-Dimensional Fermi Surfaces for the K0.25WO3 Hexagonal Bronze. Inorganic Chemistry, 2009, 48, 11492-11494. | 1.9 | 3 |
| 31 | Long-range magnetic order in the porous metalâ€“organic framework Ni(pyrazine)[Pt(CN)4]. Physical Chemistry Chemical Physics, 2017, 19, 29084-29091. | 1.3 | 3 |
| 32 | Electric field-induced oxygen vacancies in YBa2Cu3O7. Journal of Chemical Physics, 2021, 154, 224703. | 1.2 | 2 |