Publication list - Roberta Poloni

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46 publications (including Nature, Nature Chem., Nature Commun., JACS, PNAS, JPCL, JCTC)
H-index: 21
Citations: 2640 from google scholar

46. A. Martinez-Martinez, E. Resines-Urien, L. Piñeiro-López, A. Fernández-Blanco, A. L. Mariano, R. Poloni, J. Alberto Rodíguez-Velamazán, E. Carolina Sañudo, E. Burzurí, J. Sánchez Costa, *Unravelling interplay between molecule-based spin-state switching and electron transport in a single-crystal 3D metal-organic framework* Research Square submitted to JACS;

45. A. L. Mariano, A. Fernández-Blanco, R. Poloni* *Efficient Capture-and-Release Mechanism via a Spin Crossover-Mediated Change in Gas Affinity in Metal-Organic Frameworks from Ab initio Calculations* ChemRxiv 10.26434/chemrxiv-2022-7z5r5 (2022), submitted to JACS;

44. A. Fernández-Blanco, L. Piñeiro-López, M. Jiménez-Ruiz, S. Rols, J. A. Real, R. Poloni*, J. A. Rodríguez-Velamazán *CO and CO_2 Adsortpion Mechanism in Fe(pz)[Pt(CN)$_4$] Probed by Neutron Scattering and Density-Functional Theory Calculations* ChemRxiv 10.26434/chemrxiv-2022-bpfzl (2022) to be submitted;

43 A. R. Kshirsagar and R. Poloni* *Assessing the role of the Kohn-Sham density in the calculation of the low-lying Bethe-Salpeter excitation energies* ChemRxiv doi:10.26434/chemrxiv-2022-18bff (2022), accepted for publication in JPCA;

42. A. Fernández-Blanco, L. A. Mariano, L. Piñeiro-López, J. A. Real, J. Sanchez Costa, R. Poloni*, J. A. Rodríguez-Velamazán *Hidden ordered structure in the archetypical Fe(pyrazine)[Pt(CN)4] spin-crossover porous coordination compound* CrystEngComm 24, 6349 (2022);

41. A. Fernández-Blanco, L. Piñeiro-López, M. Jiménez-Ruiz, S. Rols, J. A. Real, J. A. Rodríguez-Velamazán, R. Poloni* *Probing the SO_2 adsorption mechanism in Hofmann clathrates via inelastic neutron scattering and density functional theory calculations* J. Phys. Chem. C 126, 8090 (2022);

40. J. Carnis, A.R. Kshirsagar, L. Wu, M. Dupraz, S. Labat, M. Texier, L. Favre, L. Gao, F. E. Oropeza, N. Gazit, E. Almog, A. Campos, J.S. Micha, E. J. M. Hensen, S. J. Leake, T. U. Schulli, E. Rabkin, O. Thomas, R. Poloni, Jan P. Hofmann and M.I. Richard *Twin boundary migration in an individual platinum nanocrystal during catalytic CO oxidation* Nature Commun. 12, 5385 (2021);

39. A. Develioglu, E. Resines-Urien, R. Poloni, L. Martín-Pérez, J. Sanchez-Costa, E. Burzurí *Tunable Proton Conductivity and Color in a Nonporous Coordination Polymer via Lattice Accommodation to Small Molecules* Avd. Sci. 2102619 (2021);

38. L. A. Mariano and R. Poloni* *Electric field-induced oxygen vacancies in $YBa_2Cu_3O_7$* J. Chem. Phys 154, 224703 (2021);

37. A. R. Kshirsagar, X. Blase, C. Attaccalite, and R. Poloni* *Strongly Bound Excitons in Metal–Organic Framework MOF-5: A Many-Body Perturbation Theory Study* J. Phys. Chem. Lett. 12, 4045-4051 (2021);

36. L. A. Mariano, B. Vlaisavljevich, R. Poloni* *Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes via the Hubbard U-Corrected Density* J. Chem. Theory Comput. 17, 2807 (2021);

35. A.R. Kshirsagar, C. Attaccalite, X. Blase, J. Li, R. Poloni* *Bethe–Salpeter Study of the Optical Absorption of trans and cis Azobenzene-Functionalized Metal–Organic Frameworks Using Molecular and Periodic Models* J. Phys. Chem. C 125, 7401-7412 (2021);

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33. A. Kshirsagar, G. D'Avino, X. Blase, J. Li, R. Poloni* *Accurate prediction of the S_1 excitation energy in solvated azobenzene derivatives via embedded orbital-tuned Bethe-Salpeter calculations* J. Chem. Theory and Comput. 16, 2021–2027 (2020);

32. A. Gamonal, C. Sun, A. L. Mariano, E. Fernandez-Bartolome, E. San Vicente, B. Vlaisavjevich, R. Poloni*, R. Wannemacher*, J. Cabanillas-Gonzalez, J. Sanchez-Costa *Divergent Adsorption-Dependent Luminescence Amino-Functionalized Lanthanide Metal-Organic Frameworks for Highly Sensitive NO_2 Sensors* J. Phys. Chem. Letters 11, 3362–3368 (2020);

31. E. Resines-Urien, E. Burzuri, E. Fernandez-Bartolome, M. Garcia-Tunon, P. de la Presa, R. Poloni, S.J. Teat and J. Sanchez-Costa *A switchable iron-based coordination polymer toward reversible acetonitrile electro-optical readout* Chem. Sci. 10, 6612 (2019);

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29. A. Koishi, A. Fernandez-Martinez, B. Ruta, M. Jiménez-Ruiz, R. Poloni, D. di Tommaso, F. Zontone, G. A. Waychunas and G. Montes-Hernandez *The role of impurities in the kinetic persistence of amorphous calcium carbonate : a nanoscopic dynamics view* J. Phys. Chem. C 122, 16983 (2018);

28. C. Yang, A. Kshirsagar, A. Charaf-Eddin, L. Lin and R. Poloni* *Tuning Gas Adsorption by Metal Node-Blocking in Photoresponsive Metal-Organic Frameworks* Chem. Eur. J. 24, 1 (2018), *featured as Hot Paper*;

27. A. Rodriguez-Velamazan, O. Roubeau, R. Poloni, E. Lhotel, E. Palacios, M. Gonzalez, J. A. Real *Long-range magnetic order in the porous metal-organic framework Ni(pyrazine)[Pt(CN)$_4$]* Phys. Chem. Chem. Phys. 19, 29084 (2017);

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25. M. Dupraz, R. Poloni, K. Ratter, D. Rodney, M. De Santis, B. Gilles, G. Beutier and M. Verdier *Wetting layer of copper on the tantalum (001) surface* Phys. Rev. B 94, 235427 (2016);

24. Y. Lee, R. Poloni and J. Kim *Probing Gas Adsorption in MOFs Using an Efficient Ab Initio Widom Insertion Monte Carlo Method* J. Computat. Chem. 37, 2808 (2016);

23 R. Poloni and J. Kim *Thermodynamics of gas adsorption in MOFs using ab initio calculations* Perspective article in Int. J. Quantum Chem. 116, 569 (2016);

22. W. Drisdell, R. Poloni, T. McDonald, T. Pascal, L. Wan, C. Pemmaraju, B. Vlaisavljevich, S. Odoh, J. B. Neaton, J. R. Long, D. Prendergast, J. B. Kortright *Probing the mechanism of CO_2 capture in diamine-appended metal-organic frameworks using measured and simulated X-ray spectroscopy* Phys. Chem. Chem. Phys. 17, 21448 (2015);

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20. R. Poloni*, K. Lee, R. Berger, B. Smit and J. B. Neaton *Understanding trends in CO_2 adsorption in MOFs with open-metal sites'* J. Phys. Chem. Letters 5, 861 (2014);

19. R. Poloni and J. Kim *Predicting low-k zeolite materials* J. Mater. Chemistry C 2, 2298 (2014);

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12. R. Poloni, J. Íñiguez, A. García and E. Canadell, *Efficient first-principles method for structural studies of materials with substitutional disorder*, J. Phys. Condens. Matter 22, 415401 (2010);

11. R. Poloni, E. Canadell and J.-P. Pouget *Concerning the possibility of hidden one-dimensional Fermi surfaces for the $K_{0.25}WO_3$ hexagonal bronze* Inorg. Chem. 48, 11492 (2009);

10. R. Poloni, P. Toulemonde, D. Machon, S. Le Floch, S. Pascarelli and A. San-Miguel *Amorphization of Rb_6C_{60} and Cs_6C_{60} under high temperature and high pressure conditions* High Press. Res. 29, 108 (2009);

9. S. Pasternak, G. Aquilanti, S. Pascarelli, R. Poloni, B. Canny, M.-V. Coulet and L. Zhang *A diamond anvil cell with resistive heating for high pressure and high temperature x-ray diffraction and absorption studies* Rev. Sci. Inst. 79, 085103 (2008);

8. R. Poloni, G. Aquilanti, S. Le Floch, S. Pascarelli, P. Toulemonde, D. Machon, D. Martinez-Blanco, G. Morard and A. San-Miguel *High-pressure phase transition in Rb_6C_{60}* Phys. Rev. B 77, 205433 (2008);

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5. G. Morard, C. Sanloup, G. Fiquet, M. Mezouar, N. Rey, R. Poloni and P. Beck *Structure of eutectic Fe-FeS melts to pressures up to 17 GPa: implications for planetary cores* Earth and Planetary Science Letters 263, 128 (2007);

4. G. Morard, M. Mezouar, N. Rey, R. Poloni, A. Merlen, S. Le Floch, P. Toulemonde, S. Pascarelli, A. San Miguel, C. Sanloup and G. Fiquet *Optimization of Paris-Edinburgh cell assemblies for in situ monochromatic X-ray diffraction and X-ray absorption* High Press. Res. 27, 223 (2007);

3. E. Principi, M. Minicucci, A. Di Cicco, A. Trapananti, S. De Panfilis and R. Poloni *Metastable Bi under extreme conditions investigated by combined XAS and XRD*, AIP Conf. Proceedings CP882, 532 (2007);

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