

Publication list - Roberta Poloni

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* *Adv. Sci.* **2102619** (2021);
38. L. A. Mariano and R. Poloni* *Electric field-induced oxygen vacancies in YBa₂Cu₃O₇* *J. Chem. Phys.* **154**, 224703 (2021);
37. A. R. Kshirsagar, X. Blase, C. Attacalite, 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. Vlasisavljevich, 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);
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34. L. A. Mariano, B. Vlasisavljevich, R. Poloni* *Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density-Functional Theory and the Linear-Response Hubbard U Correction* *J. Chem. Theory Comput.* **16**, 6755–6762 (2020);
33. A. Kshirsagar, G. D'Avino, X. Blase, J. Li, R. Poloni* *Accurate prediction of the S₁ 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. Vlasisavljevich, R. Poloni*, R. Wannemacher*, J. Cabanillas-Gonzalez, J. Sanchez-Costa *Divergent Adsorption-Dependent Luminescence Amino-Functionalized Lanthanide Metal-Organic Frameworks for Highly Sensitive NO₂ 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);
30. R. Poloni*, A. L. Mariano, D. Prendergast and J. Garcia-Barriocanal *Probing the electric field-induced mechanism in YBCO using computed Cu K-edge absorption spectra* *J. Chem. Phys.* **149**, 234706 (2018);
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-Velamazán, 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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19. R. Poloni and J. Kim *Predicting low-k zeolite materials* *Journal of Materials Chemistry C* **2**, 2298 (2014);
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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 Pressure Research](#) **29**, 108 (2009);
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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 Pressure Research](#) **27**, 223 (2007);
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