# Curriculum Vitae

**POLONI ROBERTA**

*Place and date of birth*: Macerata (Italy), March 4, 1979

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## Work Experience

since 10/2014: CNRS Researcher (CR1) at the Science et Ingénierie des Matériaux et Procédés laboratory (SIMaP) in Grenoble. I carry on my research on new materias (metal-organic frameworks, ionic liquids, and zeolites) for carbon capture using first-principles.

06/2013-07/2014: Associate CNRS Researcher (non permanent) at the Science et Ingénierie des Matériaux et Procédés laboratory (SIMaP) in Grenoble.

02/2010-11/2012: Postdoc with a Energy Frontier Research Center postdoctoral fellowship and joint appointment at (1) the University of California, Berkeley in the Department of Chemistry in Prof. **Berend Smit**'s group and (2) the Molecular Foundry (LBNL) in Dr. **Jeffrey B. Neaton**'s group. DFT studies applied to the following topics:

1. Engineering of metal-organic frameworks (MOFs) for $CO_2$ capture: ligand and metal substitution; amine functionalization; structural flexibility;
2. Study of binding mechanism for physisorptive and chemisorptive processeses.
3. Study of London dispersive forces in carbon capture by using van der Waals density functionals.
4. Development of classical force-field from first-principles methods (MP2 and DFT) to study carbon capture by metal-organic frameworks exhbiting open metal centers.

07/2007-12/2009: Postdoc at the Laboratory of Electronic Structure of Materials at the ICMAB (Institut de Ciència de Materials de Barcelona, Spain). DFT-based methodology:

1. Developement of an efficient computational approach based on the Virtual Crystal Approximation and DFT to determine the atomic structure of crystals with substitutional disorder. Work in collaboration with Dr. **Jorge Íñiguez** (ICMAB), Prof. **Alberto García** (ICMAB) and Prof. **Enric Canadell** (ICMAB);
2. Elastic and strain-induced properties of functional oxides (e.g. Giant Magneto-Resistance compounds) in collaboration with Dr. **Jorge Íñiguez**.
3. Structural and electronic transformation of liquid Ge and Si under high temperature and high pressure conditions by Ab-initio Molecular Dynamics. In collaboration with Prof. **Eduardo Hernández** (Instituto de Ciencia de Materiales de Madrid, Spain).

## Education

**01/09/2004–31/10/2007** : Ph.D. in Condensed Matter Physics from the University Lyon 1 (France) at the ESRF (European Synchrotron Radiation Facility, Grenoble, France) in the absorption beamline (BM29).
Supervisors: Prof. **Alfonso San Miguel** (University Lyon 1) and Dr. **Sakura Pascarelli** (ESRF).

Ph.D. Research Activities:

1. The main project included a combined experimental and theoretical study of the structural and electronic properties of some heavy alkali metal-doped fullerenes ($Rb_6C_{60}$ and $Cs_6C_{60}$) under high pressure and high temperature conditions by employing XAS (X-Ray Absorption Spectroscopy), XRD (X-Ray Diffraction), Raman Spectroscopy and DFT calculations.

   Thesis title:
   Heavy alkali metal-intercalated fulleneres under high temperature and high pressure conditions: $Rb_6C_{60}$ and $Cs_6C_{60}$.
2. Study of the structural evolution of low melting point metals under high-temperature and high-pressure conditions by using XAS and XRD techniques.
3. Geophysical problems. I worked on XRD experiments in collaboration with geophysics group in Lyon on the structure of planetary cores, and in particular on Fe-FeS melts.

**2003–2004** : M. Sc. ("Laurea") in Physics (University of Camerino, Italy), with grade 110/110 *summa cum laude*.
Supervisors: Prof. **Andrea Di Cicco** (University of Camerino) and Dr. **Simone De Panfilis** (ESRF).
I studied the evolution of the local structure of liquid gallium under high temperature and high pressure conditions by XAS and XRD.

Thesis title:
Liquid gallium in confined droplets under high temperature and high pressure conditions by EXAFS spectroscopy.

**1999–2003** : B. Sc. in Physics at the University of Camerino with grade 110/110 *summa cum laude*.

## Other activities

**Peer Review activity**:
Phyical Review B, European Physical Jounal B, Journal of Physical Chemistry C, Journal of Physical Chemistry B, Communications in Computational Physics

**Highlights**:

**1.** R. Poloni, S. De Panfilis, A. Di Cicco, G. Pratesi, E. Principi, A. Trapananti and A. Filipponi, "Liquid Gallium in Confined Droplets under High Temperature and High Pressure Conditions", European Synchrotron Radiation Facility Highlights, Highlights 2005;

**2.** R. Poloni, G. Aquilanti, S. Le Floch, M. V. Fernandez-Serra, S. De Panfilis, P. Toulemonde, D. Machon, G. Morard, D. Martinez-Blanco, W. Crichton, S. Pascarelli, A. San-Miguel, "Alkali Metal-Intercalated Fullerenes under High Pressure", European Synchrotron Radiation Facility Highlights, Highlights 2008;

**3.** A. Dzubak, L. Lin, J. Kim, J. A. Swisher, R. Poloni, S. N. Maximoff, B. Smit and L. Gagliardi, "Speeding the Search for Better Carbon Capture", Science News 2012, Science Daily; Berkeley Lab News;

**4.** W. Drisdell, R. Poloni, T. M. McDonald, J. R. Long, B. Smit, J. B. Neaton, D. G. Prendergast and J. B. Kortright, "An Inside Look at a MOF in Action", Science News 2013, Science Daily; Highlight 2013 in Phys.org; Berkeley Lab News.

## Invited talks and Conferences

"Institut of Chemistry of Clermont-Ferrand", February 2014, Clermont-Ferrand, invited talk ("First-Principles calculations of Carbon Capture");

"Institut de la Matière Condensée de Bordeaux (ICMCB)", 16/12/2013, Bordeaux, invited talk ("First-Principles calculations of Carbon Capture");

"Laboratoire de Science et Ingénierie des Matériaux et Procéd(SIMaP)", 15/03/2013, Grenoble, invited talk ("Carbon Capture by Metal-Organic Framework using First-Principles");

"Institut Néel", 13/03/2013, Grenoble, invited talk ("Carbon Capture by Metal-Organic Framework using First-Principles");

"Molecular Foundry Seminars", 5/10/2012, Berkeley, invited talk ("Carbon Capture by Metal-Organic Framework");

"Young Engineers and Scientists Symposium", 20/03/2012-22/03/2012, Berkeley, invited talk ("Enhancement of $CO_2$ capture in tunable MOFs: Balancing Electrostatic and van der Waals interactions");

"American Physical Society (APS) March Meeting 2012",26/02/2012-02/03/2012, Boston (U.S.), oral presentation ("Ligand-Assisted Enhancement of $CO_2$ capture in metal-organic frameworks");

"American Physical Society (APS) March Meeting 2011",21/03/2011-25/03/2011, Dallas (U.S.), oral presentation ("First-Principles Calculations of the Role of Dispersive Interactions in $CO_2$ binding in metal-organic frameworks");

"Computation Carbon Capture" 26/07/2010-28/07/2010, Lausanne (Switzerland), CECAM, invited talk ("First-Principles study of $CO_2$ in Metal Organic Frameworks");

"Nanoselect-Consolider", 09/07/2009-10/07/2009, Manresa (Spain), oral presentation ("First-principles methods to study oxides and oxynitrides");

"American Physical Society (APS) March Meeting 2009", 16/03/2009-20/03/2009, Pittsburgh (U.S.), oral presentation ("A VCA-based method for the study of disordered alloys and solid solutions");

"$14^{th}$ International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods", 07/01/2009-11/01/2009, Trieste (Italy), poster presentation ("A new Virtual Crystal Approximation Approach");

20/03/2009, ICMAB (Barcelona), invited talk ("Structural and electronic evolution of intercalated fullerenes under pressure");

"$46^{rd}$ EHPRG" International Conference on High Pressure Science and Technology, 07/09/2008-12/09/2008, Valencia (Spain), oral ("Alkali metal-intercalated fullerenes under extreme conditions") and poster presentations ("Elastic properties of $Zn_xHg_{1-x}Te$ pseudobinary alloys" and "Pushing, pulling, deforming and cracking fullerenes at high pressure assisted by intercalation");

"High Pressure and Synchrotron Radiation" Workshop, 08/02/2006-10/02/2006, Grenoble (France), poster presentation ("EXAFS measurements on $Rb_6C_{60}$ and $Cs_6C_{60}$ under extreme conditions");

"$20^{th}$ AIRAPT-$43^{rd}$ EHPRG" International Conference on High Pressure Science and Technology, 27/06/2005-01/07/2005, Karlsruhe (Germany), poster presentation ("Liquid Ga in confined droplets under HT-HP conditions");

"POLIMAT" Polymorphysm in Liquid and Amorphous Systems Workshop, 07/09/2004-09/09/2004, Grenoble (France), poster presentation ("Liquid Ga in confined droplets under HT-HP conditions").

## Publication list

**23** R. Poloni and J. Kim, "Thermodynamics of gas adsorption in MOFs using *ab initio* calculations", Perspective article in International Journal of Quantum Chemistry 2015 DOI: 10.1002/qua.25057;

**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" Physical Chemistry Chemical Physics 17, 21448 (2015);

**21.** T. McDonald, J. Mason, X. Kong, E. Bloch, D. Gygi, A. Dani, V. Crocell, F. Giordanino, S. Odoh, W. Drisdell, B. Vlaisavljevich, A. Dzubak, R. Poloni, S. Schnell, N. Planas, K. Lee, T. Pascal, L. Wan, D. Prendergast, J. B. Neaton, B. Smit, J. B. Kortright, L. Gagliardi, S. Bordiga, J. Reimer, J. R. Long, "Cooperative insertion of CO2 in diamine-appended metal-organic frameworks" Nature 519, 303 (2015);

**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", the Journal of Physical Chemistry Letters 5, 861 (2014);

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

**18.** W. Drisdell, R. Poloni, T. M. McDonald, J. R. Long, B. Smit, J. B. Neaton, D. G. Prendergast and J. B. Kortright, "Probing adsorption interactions in metal-organic frameworks using x-ray spectroscopy", Journal of American Chemical Society 135, 18183 (2013);

**17.** N. Planas, A. L. Dzubak, R. Poloni, L. Lin, A. McManus, T. McDonald, FJ. B. Neaton, J. R. Long, B. Smit and L. Gagliardi, "The mechanism of carbon dioxide adsorption in an alkylamine-functionalized metal-organic framework", Journal of American Chemical Society 135, 7402 (2013);

**16.** A. Dzubak, L. Lin, J. Kim, J. A. Swisher, R. Poloni, S. N. Maximoff, B. Smit and L. Gagliardi, "*Ab-initio* carbon capture in open-site metal-organic frameworks", Nature Chemistry 4, 810 (2012);

**15.** R. Poloni, B. Smit and J. B. Neaton, "$CO_2$ capture by metal-organic frameworks with van der Waals density functionals", Journal of Physical Chemistry A 116, 4957 (2012);

**14.** R. Poloni, B. Smit and J. B. Neaton, "Ligand-assisted enhancement of $CO_2$ capture in metal-organic frameworks", Journal of American Chemical Society 134, 6714 (2012);

**13.** R. Poloni, A. San Miguel and M. V. Fernandez-Serra, "A first-principles study of the effect of charge doping on the 1D polymerization of $C_{60}$", Journal of Physics: Condensed Matter 24, 095501 (2012) (highlighted issue);

**12.** R. Poloni, J. Íñiguez, A. García and E. Canadell, "Efficient first-principles method for structural studies of materials with substitutional disorder", Journal of Physics: Condensed 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", Inorganic Chemistry 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 Pressure Research 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", Review of Scientific Instrument 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 $Rb_6C_{60}$", Physical Review B 77, 205433 (2008);

**7.** R. Poloni, D. Machon, M. V. Fernandez-Serra, S. Le Floch, G. Montagnac, H. Cardon and A. San-Miguel, "High-pressure stability of $Cs_6C_{60}$", Physical Review B 77, 125413 (2008);

**6.** R. Poloni, M. V. Fernandez-Serra, S. Le Floch, S. De Panfilis, P. Toulemonde, D. Machon, W. Crichton, S. Pascarelli, and A. San-Miguel, "Pressure induced deformation of the $C_{60}$ fullerene in $Rb_6C_{60}$ and $Cs_6C_{60}$", Physical Review B 77, 035429 (2008);

**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 Pressure Research 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);

**2.** E. Principi, M. Minicucci, A. Di Cicco, A. Trapananti, S. De Panfilis and R. Poloni, "Metastable phase diagram of Bi probed by single-energy x-ray absorption detection and angular dispersive x-ray diffraction", Physical Review B 74, 064101 (2006);

**1.** R. Poloni, S. De Panfilis, A. Di Cicco , G. Pratesi, E. Principi, A. Trapananti and A. Filipponi, "Liquid gallium in confined droplets under high-temperature and high-pressure conditions", Physical Review B 71, 184111 (2005).