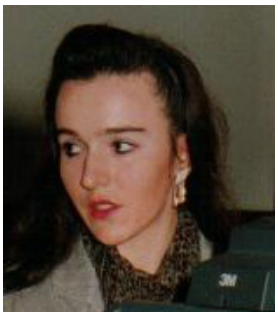
Curriculum Vitae



Prof. Giuseppina Raffaini, PhD

PERSONAL DATA

Name: Giuseppina Raffaini

Date of Birth: 23/11/1971
Place of Birth: Bergamo, Italy
Citizenship: Italian

Politecnico di Milano- Dipartimento di Chimica, Materiali e Ing. Chimica "Giulio Natta"
Phone: Office +39 (0)2 2399 3068, Laboratory: +39 (0)2 2399 30683058

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Website

EDUCATION

1997	**Degree in Chemistry** from the Università degli Studi di Milano.
1998-2000	Diploma "**Advanced School in Polymer Science G. Natta**" **at Politecnico di Milano** with the mark 100/100.
2000-2002	**Fellowship** for research activity in collaboration with proff. F.Ganazzoli and F.Montevecchi of Politecnico di Milano (CIRIC).
September 2004	**Inter-university Master in Biomaterials,** Master conferred by **CIRMIB** (*Inter-university Centre for Research on Materials for Biomedical Engineering*" www.cirmib.ing.unitn.it), supervisor: prof. Matteo Santin (University of Brighton, UK – presently President of ESB, European Society for Biomaterials).
2002-2005	**PhD in Materials Engineering at Politecnico di Milano *cum laude*** (http://ingmat.chem.polimi.it).

2005-2008 **Fellowship** for three years for research activity at Politecnico di Milano, for two years in collaboration with prof. F. Ganazzoli
for one year in collaboration with prof. A. Citterio.

June 2008-December 2014: **ASSISTANT PROFESSOR** (*Ricercatore*) at the Department of Chemistry, Materials and Chemical Engineering of the Politecnico di Milano.

In February 2014: she got the **Abilitazione Scientifica Nazionale** for the Sector "Chemical basis of technology applications" (Italian "SC 03/B2", Scientific Disciplinary Sector SSD CHIM/07) **as Associate Professor** (conferred on 17th February 2014 – valid for four years)
surpassing all the three required bibliometric parameters (Number of ISI papers, Number of citations, and contemporary H-index of the last ten years).

In December 2014 she became **ASSOCIATE PROFESSOR** (*Professore Associato*)
at the Department of Chemistry, Materials and Chemical Engineering of the Politecnico di Milano.

TEACHING AND EDUCATIONAL OUTREACH

Giuseppina Raffaini has a proven teaching experience in the basic courses of Chemistry for Engineering bachelor students at the Politecnico di Milano.

- **Since 2000**: **teaching assistant for courses of Chemistry for Engineering bachelor students** at Politecnico di Milano.
- **Since 2005**: **teacher** of courses of Chemistry for Engineering bachelor students, at Politecnico di Milano, with responsibility of evaluation in the final examination board.
- **Since the Academic Year 2010-2011 Teaching in PhD courses**: The candidate is in charge of Module 6b - Molecular Simulations of Materials B, module of a course of 2.5 credits **for the PhD program in Materials Engineering at the Politecnico di Milano**.

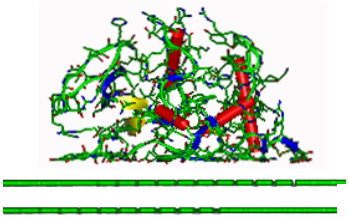
PRESENT TEACHING COURSES

In this Academic Year 2014-2015:

- as institutional teaching duty "**FONDAMENTI DI CHIMICA E CHIMICA ORGANICA**" (10 credits ECTS) **for Biomedical Engineering** (P-Z group), for the "II Scuola di Ingegneria Industriale e dell'Informazione" of the Leonardo Campus of the Politecnico di Milano.

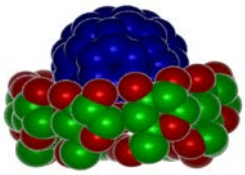
- as teaching assistant in charge of specialized seminars for "**INTRODUZIONE ALLA SCIENZA DEI MATERIALI - A**" for Materials and Nanotechnology Engineering, prof. F. Ganazzoli.

Research interests



Lysozyme on graphite

- Simulation of **biomaterials**
- **Protein adsorption**
- **Polymer surfaces**
- Wettability
- **Inclusion complexes**
- **Cyclodextrins**, nanosponges and **drug delivery**
- **Self-assembly** of modified cyclodextrins



C_{60} and γ-cyclodextrin complex

Starting her research activity in 1999, dr. Raffaini is **co-author of 37 original peer-reviewed ISI papers (H-index = 15)**, **two invited reviews which received more than 597 citations** (478 without self-citations) (source Web of Science), **4 contributions to international books, 2 contributions to national books.**

She gave **four invited lectures at National Conferences** and **three invited lectures at International Conferences**, moreover, she presented her scientific results, related both to protein adsorption on biomaterials and to inclusion complexes in several other oral and poster communications (about 38 oral communications and about 22 poster communications) at national and international meetings.

PROJECTS

Member of one operating unit in the projects:

- **PRIN** (Research Projects of National Interest) **2000**

National Coordinator prof. P. Giusti. Title of the project: **Study of the interactions between synthetic and biological systems for the realization of new biomaterials.**

- **PRIN** (Research Projects of National Interest) **2005**

National Coordinator prof. G. Marletta. Title of the project: **Self-assembling film of sintetic oligopeptides for biomimetic surfaces**.

- **FIRB** (Fund for Investments in Basic Research) – Call "Future in research" **2008**, co-financed by MURST in 2010 (RBFR08XH0H_001) "**SURFACE-ASSOCIATED SELECTIVE TRANSFECTION**" (SAST), national coordinator dr. G. Candiani.

- **PRIN (Research Projects of National Interest) 2010-2011**

National Coordinator prof. Walther Caminati. Title of the project: "Frontier studies in spectroscopy and dynamics of molecules: from simple molecular systems to supramolecular aggregates and advanced materials".

PROFESSIONAL ACTIVITIES

- Membership in Scientific Societies: ACS, ESB, SIB, Società Italiana Ciclodestrine.

- Affiliated to:
  - the Inter-University Consortium for the Science and Technology of Materials INSTM
  - the Inter-University Research Centre “The Protein Factory”.

- Group coordinator of the research team of the Italian Society of Cyclodextrins for the molecular modelling of Inclusion Complexes of Cyclodextrins at the Politecnico di Milano (web-site http://www.cdtec.unito.it/gruppo_raffaini.html).

- Referee for the journals Langmuir, J Phys Chem, Phys. Chem. Chem. Phys., Chem. Phys. Lett., Phil. Trans. Royal Soc. A, Plos One, Comput. Theor. Chem., Eur. J. Pharm. Soc., J Incl Phen. Macrocycl. Chem.

PAPERS IN INTERNATIONAL JOURNALS

(H-index 15)

[1] F. GANAZZOLI, **G. RAFFAINI**, “Non-newtonian viscosity in linear and star polymers”, *Macromol. Theory Simul*., 8, 234-246 (1999).

[2] F. GANAZZOLI, R. LA FERLA, **G. RAFFAINI** "Intramolecular dynamics of dendrimers under excluded-volume conditions", *Macromolecules*, 34, 4222-4228 (2001).

[3] S. MANTERO, D. PIURI, F. M. MONTEVECCHI, S. VESENTINI, F. GANAZZOLI, **G. RAFFAINI** "Albumin adsorption onto pyrolytic carbon: a molecular mechanics approach", *J. Biomed. Mat. Res.*, **59**, 329 (2002).

[4] F. GANAZZOLI, **G. RAFFAINI**, V. ARRIGHI “The stretched-exponential approximation to dynamic structure factor in non-entangled polymer melts”, *Physical Chemistry Chemical Phisics*, 4, 3734-3742 (2002).

[5] A. MELE, **G. RAFFAINI**, F. GANAZZOLI, A. SELVA, “β-Cyclodextrin and 5-methoxytryptammonium ion host-guest association in vacuo: simulation of

non-covalent inclusion by molecular dynamics", *J. Incl. Phenom. Macrocyclic Chem.*, 44, 219 (2002).

[6] F. GANAZZOLI, **G. RAFFAINI**, V. ARRIGHI, "The Dynamic Structure Factor in Non-entangled polymer melts – Theoretical Results for Real Chains and the Stretched Exponential Approximation", *Chem. Phys*., 287, 391 (2003), *Chem. Phys*., 292, 347 (2003).

[7] A. MELE, **G. RAFFAINI**, F. GANAZZOLI, M. JUZA,V. SCHURIG, "Macrocycle conformation and self-inclusion phenomena in octakis(3-O-butanoyl-2,6-di-O-n-pentyl)-γ-cyclodextrin (Lipodex E) by NMR spectroscopy and molecular dynamics", *Carbohydrate Res*. 338, 625 (2003).

[8] **G. RAFFAINI**, F. GANAZZOLI, "A simulation study of the interaction of some albumin sub–domains with a flat graphite surface", *Langmuir*, 19, 3403 (2003).

[9] **G. RAFFAINI**, F. GANAZZOLI, "Molecular Dynamics Simulation of the Adsorption of a Fibronectin Module on a Graphite Surface", *Langmuir*, 20, 3371 (2004).

[10] **G. RAFFAINI**, F. GANAZZOLI, "Surface ordering of proteins adsorbed on graphite", *J. Phys. Chem. B*, 108 (36), 13850-13854 (2004)

[11] T. HAACK, R. FATTORI, M. NAPOLETANO, F. PELLACINI, G. FRONZA, **G. RAFFAINI**, F. GANAZZOLI, Phthalazine PDE IV Inhibitors. Conformational Study of some 6-methoxy-1,4-Disubstituted Derivatives, *Bioorg. Med. Chem.*, **13**, *4425* (2005).

[12] **G. RAFFAINI**, F. GANAZZOLI, Adsorption of charged albumin subdomains on a graphite surface, *J. Biomed. Mat. Res. A*, **76**, *638* (2006).

[13] **G. RAFFAINI**, S. ELLI, F. GANAZZOLI, Computer simulation of bulk and surface properties of biomaterials, *J. Biomed. Mat. Res. A*, 77, 618 (2006).

[14] **G. RAFFAINI**, F. GANAZZOLI, Protein Adsorption on the Hydrophilic Surface of a Glassy Polymer: a Computer Simulation Study, *Phys. Chem. Chem. Phys.*, **8**, *2765* (2006).

[15] **G. RAFFAINI***, F. GANAZZOLI, Molecular dynamics study of host-guest interactions in cyclodextrins: methodology and data analysis for a comparison with solution data and the solid state structure, *J. Incl. Phenom. Macrocyclic Chem.*, ***special issue,* 57**, 683 (2007).

[16] **G. RAFFAINI***, F. GANAZZOLI, Hydration and flexibility of α-, β-, γ- and δ-cyclodextrin: a molecular dynamics study, *Chem. Phys.*, **333**, 128 (2007).

[17] **G. RAFFAINI**, F. GANAZZOLI, Sequential Adsorption of Proteins and the Surface Modification of Biomaterials: a Molecular Dynamics Study, *J. Mater. Sci. - Mater. Med.*, ***special issue, invited article***, **18**, 309 (2007).

[18] S. ELLI, **G. RAFFAINI**, F. GANAZZOLI, E. G. TIMOSHENKO, YU. A. KUZNETSOV, Surface adsorption of comb polymers by Monte Carlo simulations, *Polymer*, 49, 1716 (2008).

[19] M. ORMELLESE, E.A. PÉREZ, **G. RAFFAINI**, F. GANAZZOLI, L. LAZZARI, Inhibition mechanism in concrete by organic substances: an experimental and theoretical study, *NACE Corrosion Conference* 2009, Atlanta (USA), paper 09221, pp. 1–19. ©2009 NACE, Houston.

[20] **G. RAFFAINI***, F. GANAZZOLI, L. MALPEZZI, C. FUGANTI, G. FRONZA, W. PANZERI, A. MELE, Validating a strategy for molecular dynamics simulations of cyclodextrin inclusion complexes through single-crystal X-ray and NMR experimental data: a case study. *J. Phys. Chem. B* , **113**, 9110–9122 (2009).

[21] **G. RAFFAINI***, F. GANAZZOLI, Surface Hydration of Polymeric (Bio)Materials: a Molecular Dynamics Simulation Study, *J. Biomed. Mat. Res. A*, **92**, *1382–1391* (2010).

[22] **G. RAFFAINI***, F. GANAZZOLI, Protein adsorption on a hydrophobic surface: a molecular dynamics study of lysozyme on graphite, *Langmuir* , **26**: 5679-5689 (2010)

[23] **G. RAFFAINI***, F. GANAZZOLI, A Molecular Dynamics Study of the Inclusion Complexes of C_{60} with Some Cyclodextrins *J. Phys. Chem. B* , **114**, 7133–7139 (2010)

[24] M. ORMELLESE, E. A. PÉREZ, **G. RAFFAINI**, F. GANAZZOLI, L. LAZZARI, Inhibition mechanism in concrete by organic substances: an experimental and theoretical study, *J. Mat. Sci. Eng.*, **4**, *66-77* (2010).

[25] **G. RAFFAINI**, F. GANAZZOLI, Protein adsorption on biomaterial and nanomaterial surfaces: a molecular modeling approach to study non-covalent interactions, *J. Appl. Biomater. Biomech.*,Vol. **8**, n°3, pp. 135-145 (2010).

[26] A. MELE, F. CASTIGLIONE, L. MALPEZZI, F. GANAZZOLI, **G. RAFFAINI**, F. TROTTA, B. ROSSI, A. FONTANA, G. GIUNCHI, "HR MAS NMR, powder XRD and Raman spectrocopy study of inclusion phenomena in β-CD nanosponges", *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **69**, 403-409 (2011).

[27] M.C.Tanzi, S.Bozzini, G.Candiani, A.Cigada, L.DeNardo, S.Farè, F.Ganazzoli, D.Gastaldi, M.Levi, P.Metrangolo, F.Migliavacca, R.Osellame, P.Petrini, **G.RAFFAINI**, G.Resnati, P.Vena, S.Vesentini and P.Zunino, Smart Biomaterials and Drug Delivery at Politecnico di Milano, *J. Appl. Biomater. Biomech.*, Vol. 9 no. 2, 87-97**,** (2011).

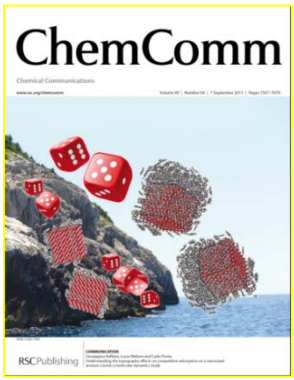
[28] **G. RAFFAINI**, F. GANAZZOLI, Molecular modeling study of protein adsorption on the surface of titanium dioxide polymorphs, *Phil. Trans. R. Soc. A* 2012 370, 1444-1462 (2012), ***invited article***.

[29] L. DE NARDO, **G. RAFFAINI**, E. EBRAMZADEH, F. GANAZZOLI, Titanium oxide modeling and design for innovative biomedical surfaces: a concise review, *Int J Artif Organs*; 35 (9): 629-641 (2012).

[30] **G. RAFFAINI***, F. GANAZZOLI, A molecular modeling study of complex formation and selfaggregation behavior of a porphyrin–beta-cyclodextrin conjugate, *J Incl Phenom Macrocycl Chem*, **76**, pp. 213–221 (2013)

[31] **G. RAFFAINI**, F. GANAZZOLI, A. MELE, F. CASTIGLIONE, A molecular dynamics study of cyclodextrin nanosponge models, *J Incl Phenom Macrocycl Chem* 75:263–268 (2013).

[32] **G. RAFFAINI***, F. GANAZZOLI, Surface Topography Effects in Protein Adsorption on Nanostructured Carbon Allotropes, *Langmuir*, 29, 4883−4893 (2013).



[33] **G. RAFFAINI***, L. MELONE, C. PUNTA, Understanding the topography effects on competitive adsorption on a nanosized anatase crystal: a molecular dynamics study *Chem. Commun*, **49**, pp. 7567- 7570 (2013). ***Inside Cover.***

[34] **G. RAFFAINI**, "Modellazione molecolare dell'adsorbimento di proteine su polimorfi di TiO_2", 150° Convegno Nazionale, articolo n° 37 ISBN 978 88 6493 0213.

[35] **G. RAFFAINI***, A. MAZZAGLIA, F. GANAZZOLI, Aggregation behaviour of amphiphilic cyclodextrins: the nucleation stage by atomistic molecular dynamics, *Journal of Organic Chemistry*, **11**, pp. 2459-2473 (2015).

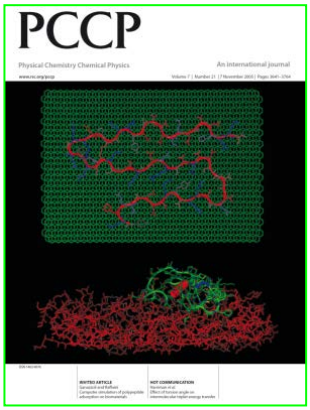
[36] M.V. DIAMANTI*, E.A. PÉREZ ROSALES, **G. RAFFAINI***, F. GANAZZOLI, A. BRENNA, M. PEDEFERRI, M. ORMELLESE, Molecular modelling and electrochemical evaluation of organic inhibitors in concrete, *Corrosion Science*, **100**, pp. 231-241 (2015).

[37] **G. RAFFAINI***, F. GANAZZOLI, Separation of chiral nanotubes with an opposite handedness by chiral oligopeptide adsorption: A molecular dynamics study, *Journal of Chromatography A*, **1425**, pp. 221-230 (2015).

[38] **G. RAFFAINI***, F. GANAZZOLI, A. MAZZAGLIA, Aggregation behavior of amphiphilic cyclodextrins in a nonpolar solvent: evidence of large-scale structures by atomistic molecular dynamics simulations and solution studies, *Journal of Organic Chemistry*, **12**, pp. 73-80 (2016).

[39] **G. RAFFAINI*,** R. MILANI*, F. GANAZZOLI, G. RESNATI, P. METRANGOLO*, Atomistic simulation of hydrophobin HFBII conformation in aqueous and fluorous media and at the water/*vacuum* interface, *Journal of Molecular Graphics and Modelling*, **63**, pp. 8-14 (2016).

INVITED REVIEWS



[1] **G. RAFFAINI**, F. GANAZZOLI Computer simulation of polypeptide adsorption on biomaterials, *Phys. Chem., Chem. Phys.*, **7**, *3651* (2005), ***invited review*** (*inside cover*).

[2] **G. RAFFAINI**, F. GANAZZOLI, Understanding the performance of biomaterials through molecular modeling: crossing the bridge between their intrinsic properties and the surface adsorption of proteins, *Macromol. Biosci.*, ***special issue, invited paper***, **7**, 552 (2007).

BOOK CHAPTERS

International books

[1] **G. RAFFAINI**, F. GANAZZOLI, "Protein adsorption on a hydrophobic graphite surface", in *Computer Simulations Bridging Liquid Crystals and Polymers*, Editori P. Pasini, C. Zannoni, S. Žumer, *NATO Science Series II*, Kluwer Academic Publishers, Dordrecht, Vol. 177, p. 203 (2004).

[2] L. De Nardo, **G. Raffaini**, F. Ganazzoli, R. Chiesa, Metal surface oxidation and surface interactions, in "Surface modification of biomaterials: methods, analysis and applications", Ed. R. Williams, Woodhead (Cambridge, UK), ISBN 1845696409 pp. 102 – 142 (2011).

[3] C. Gambarotti, L. Melone, C. Punta, **G. Raffaini**, Photocatalytic Minisci Reaction: A Promising and Eco-friendly Route to Functionalize Heteroaromatics of Biological Interest in Green Synthetic Approaches for Biologically Relevanteterocycles. G. Brahmachari, Ed. 2014, Elsevier.

National books

[4] F. Ganazzoli, **G. Raffaini**, Simulazione molecolare dell'adsorbimento di proteine su superfici, in "Biomateriali: dagli impianti protesici alla medicina rigenerativa", Editori A. Cigada, R. Contro, C. Di Bello, M. C. Tanzi, Patron Editore, Bologna (2005).

[5] F. Ganazzoli, **G. Raffaini**, "Termodinamica statistica di polimeri in soluzione", XXXV Convegno-Scuola AIM 19-23 maggio 2014, Gargnano (BS). Capitolo di libro.

PROCEEDINGS

[1] A. MELE, **G. RAFFAINI**, M. JUZA, V. SCHURIG, "Conformational properties of octakis(3-o-butanoyl-2,6-di-o-n-pentyl)-γ-cyclodextrin (Lipodex E) and its mode of interaction with the inhalation anaesthetic enflurane. An NMR and molecular dynamics study". *Proceedings of 10th International Cyclodextrin Symposium*, May 21-24 (2000), Ann Arbor, Michigan, USA, pp. 149-156.

[2] **G. RAFFAINI**, F. GANAZZOLI, "Atomistic simulations of protein adsorption on graphite", in "*Science and Supercomputing at CINECA*", 2003 report, CINECA, Bologna. Versione on-line: http://www.cineca.it/editions/ssc2003/2003/chi13.pdf.

[3] **G. RAFFAINI**, F. GANAZZOLI, Molecular Simulations of Proteins Adsorbed on Biomaterials and on Carbon Nanotubes, *J. Appl. Biomat. Biomech.* **2**, *214* (2004).

[4] **G. Raffaini**, F. Ganazzoli, Interazione di proteine con nanotubi di carbonio a singola parete e fullereni, *Proceedings VIII Congresso Nazionale AIMAT* (Palermo, 27 giugno-1°luglio 2006), Atti su cd.

[5] L. MALPEZZI, F. CASTIGLIONE, F. GANAZZOLI, A. MELE, W. PANZERI, **G. RAFFAINI**, The inclusion complexes of β-cyclodextrin with tricyclic drugs: an X-ray diffraction, NMR and Molecular Dynamics study, *Proceedings 14th International Cyclodextrins Symposium*, Kyoto (Giappone), 8-11 maggio 2008.

[6] M.V. Diamanti, M. Ormellese, E.A. Pérez-Rosales, M. Pedeferri, **G. RAFFAINI**, F. Ganazzoli, An experimental and theoretical study of the inhibition mechanism of organic substances in concrete, in "Nanotechnology 2010: Advanced Materials, CNTs, Particles, Films and Composites", proceedings of Nanotech Conference & Expo 2010, Anaheim, CA, CRC Press, ISBN 9781439834015, pp. 689-692 (2010).

[7] **G. RAFFAINI**, F. Ganazzoli, Molecular Modeling of Protein Adsorption at Biointerfaces: Surface Modification and Nanostructure for Smart Biomaterials, Proceedings "BioMed@POLIMI: 20 yrs and beyond", Milano, 30th November 2010, *Smart Bio–Materials and Drug Delivery* Paper N. 05_8 – pp. 179-182.