Curriculum Vitae of Carlo Cavallotti

General data:

name:	Carlo Cavallotti
birth date:	Milano, July 17 1971
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Training and education

- 1995, Laurea (5 years degree) in Chemical Engineering (grade 100/100 cum laude) at Politecnico di Milano, Italy.
- 2000, Dottorato di ricerca (Ph.D.) in Chemical Engineering at Politecnico di Milano, Italy under the advisorship of Prof. S. Carrà and M. Masi. Thesis title: 'Chemical Engineering aspects in material synthesis by gas phase deposition'

Professional experiences

- September 1999 – September 2006: Assistant professor in applied physical chemistry at Dept. Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Italy.
- September 2006 – now: Associate professor of Chemical Engineering Principles at Dept. Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Italy.

International Fellowshisps

- March 1998-October 1998: visiting student in the research group of prof. K. F. Jensen at the Massachusetts Institute of Technology.
- March 2000-March 2001: post-doctoral associate fellow in the research group of prof. K. F. Jensen at the Massachusetts Institute of Technology.
- March 2016 - November 2016: Visiting Scientist at Argonne National Laboratories, Lemont, IL.

Teaching Activities

Undergraduate/Master level classes (all given at Politecnico di Milano)

1998/1999-2000/2001: practicals for the class 'Chemical Engineering Thermodynamics' for Chemical Engineering undergraduate classes.

2002/2003-2017/2018: teacher of "Applied Chemical Kinetics" at the first year of the master level degree in Chemical Engineering.

2005/2006-2013/2014: teacher of "Thermodynamics" at the first year of the master level degree in Safety Engineering (IPSIP).

2014/2015: teacher of the class "Thin solid films' at the first year of the master level degree in Chemical Engineering/Materials Engineering.

2016/2017-2017/2018: teacher of "Molecular Modeling for Chemical Engineers" at the first year of the master level degree in Chemical Engineering.

Graduate classes (all given at Politecnico di Milano)

2005/2006- 2016/2017 (every two years) PhD level course on 'Molecular Modeling', co-taught together with prof. Antonino Famulari and Guido Raos.

Awards and Recognitions

- 1994/5: winner of the 'Fondazione Famiglia Legnanese' prize for academic excellence.
- 2000: XII Italian National Award "Federchimica - per un futuro intelligente".
- 2008: selected by the most important Italian national academy, Accademia dei Lincei, and by the Inter Academy Panel (IAP) to represent Italy at the World Economic Forum in the session devoted to Young Scientists.
- 2010: invited to join the Global Young Academy, a world academy collecting top young scientists with the aim 'to unlock the potential of young scientists from around the world' https://globalyoungacademy.net/)

Editorial Activity:

- Member of the editorial board for Polymers (MDPI) from 12/2009 to 03/2018
- Member of the editorial board for International Journal of Chemical Kinetics (Wiley): from 01/2013 to 12/2015,
- Member of the editorial board for The open Crystallography Journal (Bentham Science) from 12/2009 to 11/2012

Invited presentations and keynote lectures

- ASME Pressure Vessels and Piping Conference, August 4-8, 2002 Vancouver, Canada. Invited lecture entitled: "Multiscale and multi-hierarchy modeling in electronic materials".
- Accademia nazionale dei lincei, 2-3 October 2002, "Crystal growth: from basic to applied", Roma, Palazzo Corsini. Invited lecture: "CVD: multiscale study of the selective deposition of AlGaAs".
- EuroInterFinish 2003, "Nanotechnology and coatings for novel applications" Padova, 23-24 Ottobre 2003. Invited Lecture entitled: "Material computation towards technological impact: thin solid films".
- 4th International workshop on "Modeling in Crystal Growth", Fukuoka, Japan, November 4-7, 2003. Keynote lecture entitled: "A combined 3 dimensional kinetic Monte Carlo and Quantum Chemistry study of the CVD of Si on Si (100) surfaces".
- Mini-Workshop on "Multiscale modeling in Epitaxial Growth" at the Mathematisches Forschinsinstitut Oberwolfach, January 18-24, 2004. Invited lecture entitled: "A Multiscale study of the Epitaxial CVD of Si from Chlorosilanes".
- Accademia dei Lincei, Roma, 8 Novembre 2005, German-Italian meeting 'Current issues in crystal growth from the vapor' Invited lecture entitled: 'PECVD modeling of thin films deposition'
- Workshop "Low Dimensional Dynamical Phenomena and Simulations", Erice, at the international school on solid state physics 27/7/2007. Invited Lecture entitled 'Multiscale modeling of chemical vapor deposition'
- "Multi Scale Simulations of Epitaxial Growth", invited talk presented by C. Cavallotti at the DGKK kinetic seminar of the German Association for Crystal Growth and at the IKZ at Berlin, 12-15 March 2008
- "A Multiscale Model of the Low-Temperature CVD of Si and ncSi", invited talk presented by C. Cavallotti at the 214th ECS Meeting - Honolulu, HI, October 12 - October 17, 2008.

- "Modeling the plasma CVD of nanocrystalline silicon at different length scales", invited talk presented at the European Material Research Society meeting, Strasbourg, 11 June 2010
- "Si deposition from silanes and chlorosilanes: from ab initio to reactor scale simulations of the growth process", invited talk presented at the China PV Technology International Conference (CPTIC 2012) Shanghai, 23 March 2012.
- "Molecular Modeling of the Affinity Chromatography of Monoclonal Antibodies", invited talk presented at the eight annual PEGS meeting, Boston, 4 May 2012.
- "Molecular Models of the Antibody Purification Process: from a posteriori interpretations to a priori predictions", invited talk presented at the 6th World Antibody Manufacturing Summit meeting, London, 20th September 2012.
- "Molecular Modeling of the Affinity Chromatography of Proteins: Status and Perspectives", Plenary lecture at the SPICA meeting, Bruxelles, 3 October 2012.
- "A Systematic Approach to Investigate Potential Energy Surfaces of Reacting Systems", invited talk at the TSRC Workshop: Advanced Methods for De Novo Prediction of Chemical Reaction Networks, Telluride, CO, 25-28 July 2016.
- "Recent advancements in the automation of CVD reactors for the epitaxial deposition of Si and SiC: synergy between modeling and experiments", invited talk at the Italian Crystal Growth 2017 conference, 21 November 2017.
- "Modeling the reactivity of cold plasmas", invited talk at the Workshop 'Cold Plasmas for energy and the environment', university of Trento, Italy, 24 November 2017.
- "Process analysis of non-thermal plasma assisted conversion of gaseous streams", invited talk at the international conference 'Classical and Quantum Plasmas: Matter Under Extreme Conditions' ACCADEMIA NAZIONALE DEI LINCEI e FONDAZIONE «GUIDO DONEGANI, Roma, 5-6 April 2018.
- "Coupling Automation of Single Well Rate Constant Estimation with the Investigation of Multiple Well Potential Energy Surfaces", invited talk at the fall meeting of the America Chemical Society, Boston, 19-23 August, Boston.

Other presentations at international conferences/workshops/meetings: more than 50 given in first person between 1997 and 2018.

Supervised Master thesis: more than 50.

Supervised PhD thesis/post-doc Scholars (13): Davide Moscatelli, Maurizio Rondanini, Davide Moiani, Laura Zamolo, Tommaso Casalini, Alessandro Barbato, Daniela Polino, Matteo Salvalaglio, Stefano Ravasio, Kalyan Shar, Matteo Paloni; post-docs: Tamara Moiseev; Anna Antonicci;

Participation to national/international research projects (about 1000 keuro of financial support from EU/national agencies)

- Nanophoto, Strep project, Sixth framework programme, priority 3-NMP, 'Nanocrystalline silicon films for photovoltaic and optoelectronic applications', proposal/contract no: 013944; 2005-2009. 280 keuro. (principal investigator)
- Aims, IP project, Sixth framework programme, priority 'Nanotechnology and Nanoscience', 'advanced interactive materials by design', proposal/contract no.: IP 500160-2 AIMs; 2004-2009. 310 keuro. (principal investigator)

- Simbad, Cariplo foundation project; 'Simulation, diagnostic and Modeling of an innovative CVD process, activated by low-energy-high density plasmas'. 2006-2008. 53 keuro (principal investigator)
- COST project "Unfolding Structure and Energetics of Guanidinium Binding: The Anatomy of an Important Supramolecular Anchor Group by Concerted Theoretical and Experimental Approaches" (D31/0018/05); 2006-2009. (principal investigator)
- Molecular design of selective membranes for biomolecules purification, relevant national research project program, PRIN 2008; protocol number 20085M2L3T_004; (March 2010-March 2012) 43 keuro (principal investigator)
- Coordinator and promoter of Laboratory of Molecular Modeling at Politecnico di Milano. 100 keuro (2016).
- SemI40. Power Semiconductor and Electronics Manufacturing 4.0. ECSEL-IA 692466-2 (2016-2019). Horizon 2020.165 keuro. (local unit coordinator).
- External member of the Exascale Computing Project (ECP), Project Number: 17-SC-20-SC, a collaborative effort of two DOE organizations, the Office of Science and the National Nuclear Security Administration.

Participation to research projects funded by private companies as principal investigator (about 600 keuro of financial support).

- 'Ab initio PFOA alternative surfactants characterization', Solvay Selexis; 20 keuro, 2007-2008.
- 'Innovative Technologies for the valorisation of stranded gases', ENI; 183 keuro, 2008-2009.
- 'Heavy oil upgrading using Plasmas', ENI; 250 keuro. 2009-2010.
- 'Optimization of Silicon deposition in Siemens reactors', Memc; 50 keuro 2008-2010.
- 'Processing of gases using non thermal plasmas', ENI; 65 keuro, 2016.

Research interest

The research interests of Carlo Cavallotti are focused on chemical kinetics and chemical reaction engineering. In particular he is interested in the gas phase kinetics of hydrocarbons in combustion and plasmas, in the gas phase and surface chemistry responsible for the growth of advanced materials, and in the study of biomolecular interactions. The aim of these studies is to understand qualitatively and quantitatively the kinetics and the underlying thermodynamics that is active in the investigated processes, and to exploit the knowledge so obtained in order to design new or improved processes. The approach relies on the use of quantum mechanical and molecular dynamics simulations to determine parameters that are needed to perform reactor scale simulations, for example using computational fluid dynamics or Kinetic Monte Carlo simulations. The variety of the adopted approaches allows to develop efficient multiscale models that can be used to study the considered problem at the proper length scale. Thus, elementary and multiple well reactions are studied using quantum chemistry and master equation simulations, while binding between biomolecules is investigated using molecular dynamics simulations, and plasma or chemical vapor deposition reactors are modelled using finite element models and kinetic Monte Carlo simulations to study the morphological evolution of surfaces. To reach these goals both home-made (master equation stochastic solver; 2D finite element model of plasma discharge; rate constants estimation software) and literature softwares are used.

Publications
Papers on ISI journals: 108.
Book Chapters: 15
Total citations (Google Scholar): 2319
Google Hirsch Index: 29.

List of ISI Papers

1. Pelucchi, M.; Cavallotti, C.; Faravelli, T.; Klippenstein, S.J. H-Abstraction reactions by OH, HO 2, O, O 2 and benzyl radical addition to O 2 and their implications for kinetic modelling of toluene oxidation (2018) Physical Chemistry Chemical Physics, 20(16), 10607-10627
2. Leon-Garzon, A.R.; Dotelli, G.; Villa, A.; Barbieri, L.; Gondola, M.; Cavallotti, C. Thermodynamic analysis of the degradation of polyethylene subjected to internal partial discharges (2018) Chemical Engineering Science, 180, 1-10.
3. Gao, Y.; Takahashi, M.; Cavallotti, C.; Raos, G. Molecular dynamics simulation of metallic impurity diffusion in liquid lead-bismuth eutectic (LBE) (2018) Journal of Nuclear Materials, 501, 253-260.
4. Paloni, M.; Cavallotti, C. Molecular Modeling of the Interaction of Protein L with Antibodies (2017) ACS Omega 2(10), 6464-6472.
5. Tong, H.-F.; Cavallotti, C.; Yao, S.-J.; Lin, D.-Q. Molecular insight into protein binding orientations and interaction modes on hydrophobic charge-induction resin (2017) Journal of Chromatography A, 1512, 32-42.
6. Caracciolo, A.; Vanuzzo, G.; Balucani, N.; Stranges, D.; Cavallotti, C.; Casavecchia, P. Observation of H displacement and H2 elimination channels in the reaction of O (3 P) with 1-butene from crossed beams and theoretical studies (2017) Chemical Physics Letters , 683, 105-111.
7. Gimondi, I., Cavallotti, C., Vanuzzo, G., Balucani, N., Casavecchia, P. Reaction Dynamics of O(3P) + Propyne: II. Primary Products, Branching Ratios, and Role of Intersystem Crossing from Ab Initio Coupled Triplet/Singlet Potential Energy Surfaces and Statistical Calculations (2016) Journal of Physical Chemistry A, 120 (27), pp. 4619-4633.
8. Pelucchi, M.; Cavallotti, C.; Ranzi, E.: Frassoldati, A.; Faravelli, T. Relative Reactivity of Oxygenated Fuels: Alcohols, Aldehydes, Ketones, and Methyl Esters (2016) Energy & Fuels, 30, 8665-8679.
9. Baggioli, A.; Cavallotti, C.; Famulari, A. Exploring short intramolecular interactions in alkylaromatic substrates (2016), Phys. Chem. Chem. Phys. 18, 29616-29628
10. Vanuzzo, G., Balucani, N., Leonori, F., Stranges, D., Nevrly, V., Falcinelli, S., Bergeat, A., Casavecchia, P., Cavallotti, C. Reaction Dynamics of O(3P) + Propyne: I. Primary Products, Branching Ratios, and Role of Intersystem Crossing from Crossed Molecular Beam Experiments (2016) Journal of Physical Chemistry A, 120 (27), pp. 4603-4618.
11. Vanuzzo, G., Balucani, N., Leonori, F., Stranges, D., Falcinelli, S., Bergeat, A., Casavecchia, P., Gimondi, I., Cavallotti, C. Isomer-Specific Chemistry in the Propyne and Allene Reactions with Oxygen Atoms: CH_3CH + CO versus CH_2CH_2 + CO Products (2016) Journal of Physical Chemistry Letters, 7 (6), pp. 1010-1015.
12. Gao, Y., Raos, G., Cavallotti, C., Takahashi, M. Molecular Dynamics Simulation on Physical Properties of Liquid Lead, Bismuth and Lead-bismuth Eutectic (LBE) (2016) Procedia Engineering, 157, pp. 214-221.
13. Momose, T.; Kamiya, T.; Suzuki, Y.; Ravasio, S.; Cavallotti, C.; Sugiyama, M.; Shimogaki, Y. (2016) Kinetic Analysis of GaN-MOVPE via Thickness Profiles in the Gas Flow Direction with

Systematically Varied Growth Conditions, ECS Journal of Solid State Science and Technology 5, 164-171.
14. Salvalaglio, M.; Paloni, M.; Guelat, B.; Morbidelli, M.; Cavallotti, C. (2015) A two level hierarchical model of protein retention in ion exchange chromatography, Journal of Chromatography A 1411, 50-62.
15. Persico, F.; Sansotera, M.; Bianchi, C.L.; Cavallotti, C.; Navarrini, W. (2015) Photocatalytic activity of TiO_2-embedded fluorinated transparent coating for oxidation of hydrosoluble pollutants in turbid suspensions, Applied Catalysis B: Environmental 170, 83-89.
16. Ranzi, E.; Cavallotti, C.; Cuoci, A.; Frassoldati, A.; Pelucchi, M.; Faravelli, T. (2015) New reaction classes in the kinetic modeling of low temperature oxidation of n-alkanes, Combustion and flame 162, 1679-1691.
17. Leonori, F.; Balucani, N.; Nevrly, V.; Bergeat, A.; Falcinelli, S.; Vanuzzo, G.; Casavecchia, P.; Cavallotti, C. Experimental and Theoretical Studies on the Dynamics of the O(3P)+Propene Reaction: Primary Products, Branching Ratios, and Role of Intersystem Crossing (2015) J. Phys. Chem. C 119, 14632-14652.
18. Ravasio, S.; Momose, T.; Fujii, K.; Shimogaki, Y.; Sugiyama, M.; Cavallotti, C. (2015) Analysis of the Gas Phase Kinetics active during GaN deposition from NH_3 and $Ga(CH_3)_3$ J. Phys. Chem. A 119, 7858-7871.
19. Paloni, M.; Cavallotti, C. Molecular Modeling of the Affinity Chromatography of Monoclonal Antibodies, Affinity Chromatography: Methods and Protocols (2015) 321-335.
20. Cavallotti, C.; Rossi, F.; Ravasio, S.; Masi, M. A Kinetic Analysis of the Growth and Doping Kinetics of the SiC Chemical Vapor Deposition Process (2014) Industrial & Engineering Chemistry Research, vol. 53, p. 9076-9087, ISSN: 0888-5885, doi: 10.1021/ie403907w
21. Djokic, M.R.; Van Geem, K.M.; Cavallotti, C.; Frassoldati, A.; Ranzi, E.; Marin, G.B. An experimental and kinetic modeling study of cyclopentadiene pyrolysis: First growth of polycyclic aromatic hydrocarbons (2014) Combustion And Flame, vol. 161, p. 2739-2751
22. Pelucchi, M.; Bissoli, M.; Cavallotti, C.; Cuoci, A.; Faravelli, T.; Frassoldati, A.; Ranzi, E.; Stagni, A. (2014). Improved Kinetic Model of the Low-Temperature Oxidation of n-Heptane. Energy & Fuels, vol. 28, p. 7178-7193
23. Dhar, K.; Cavallotti, C. Investigation of the Initial Steps of the Electrochemical Reduction of CO2on Pt Electrodes (2014) J. Phys. Chem. A, vol. 118, p. 8676-8688
24. Masi, M.; Cavallotti, C.; Boccalari, D.; Castellana, F. Preliminary design of a novel high throughput CVD reactor for photovoltaic applications (2014) Crystal Research and Technology, vol. 49, p. 614-619
25. Cavallotti, C.; Leonori, F.; Balucani, N.; Nevrly, V.; Bergeat, A.; Falcinelli, S.; Vanuzzo, G.; Casavecchia, P. (2014). Relevance of the Channel Leading to Formaldehyde + Triplet Ethylidene in the $O(^3P)$ + Propene Reaction under Combustion Conditions. J. Phys. Chem. Lett., vol. 5, p. 4213-4218
26. Ravasio, S.; Masi, M.; Cavallotti, C. Analysis of the Gas Phase Reactivity of Chlorosilanes (2013). J. Phys. Chem. A, vol. 117, p. 5221-5231
27. Cavallotti, P.L.; Magagnin, L.; Cavallotti, C. Influence of added elements on autocatalytic chemical deposition electroless NiP (2013) Electrochimica Acta, vol. 114, p. 805-812
28. Cavallotti, C.; Polino, D. On the kinetics of the C_5H_5 + C_5H_5 reaction (2013) Proceedings of the Combustion Institute, vol. 34, p. 557-564, ISSN: 1540-7489
29. Barker Hemings, E.; Cavallotti, C.; Cuoci, A.; Faravelli, T.; Ranzi, E. A Detailed Kinetic Study of Pyrolysis and Oxidation of Glycerol (Propane-1,2,3-triol) (2012) Combustion Science And Technology, vol. 184, p. 1164-1178
30. Cavallotti, C.; Polino, D.; Frassoldati, A.; Ranzi, E. Analysis of Some Reaction Pathways Active during Cyclopentadiene Pyrolysis (2012) J. Phys. Chem. A, vol. 116, p. 3313-3324

31. Ravasio S., Cavallotti C. Analysis of reactivity and energy efficiency of methane conversion through non thermal plasmas (2012) Chemical Engineering Science, vol. 84, p. 580-590
32. Cuccato, D.; Dossi, M.; Polino, D.; Cavallotti, C.; Moscatelli, D. Is Quantum Tunneling relevant in Free Radical Polymerization? (2012) Macromolecular Reaction Engineering, vol. 6, p. 496-506
33. Salvalaglio M., Cavallotti C. (2012). Molecular modeling to rationalize ligand-support interactions in affinity chromatography. Journal Of Separation Science, vol. 35, p. 7-19
34. Cavallotti, C.; Salvalaglio, M. Molecular modelling of the affinity chromatography of proteins: Status and perspectives (2012) Chimica Oggi-Chemistry Today, vol. 30, p. 16-19
35. Ferrara, C.; Preda, M.; Cavallotti, C. On the streamer propagation in methane plasma discharges (2012) Journal of Applied Physics, vol. 112, p. 113301-1-13301-12
36. Polino, D.; Famulari, A.; Cavallotti, C. Analysis of the Reactivity on the C_7H_6 Potential Energy Surface (2011) J. Phys. Chem. A, vol. 115, p. 7928-7936
37. Moscatelli, D.; Dossi, M.; Cavallotti, C.; Storti, G. Density Functional Theory Study of Addition Reactions of Carbon-Centered Radicals to Alkenes (2011) J. Phys. Chem. A, vol. 115, p. 52-62
38. Casalini, T.; Salvalaglio, M.; Perale, G.; Masi, M.; Cavallotti, C. Diffusion and Aggregation of Sodium Fluorescein in Aqueous Solutions (2011) J. Phys. Chem. B, vol. 115, p. 12896-12904
39. Polino, D.; Cavallotti, C. Fulvenallene Decomposition Kinetics (2011) J. Phys. Chem. A, vol. 115, p. 10281-10289
40. Cavallotti, C.; Masi, M. Kinetics of $SiHCl_3$ Chemical Vapor Deposition and Fluid Dynamic Simulations. Journal of Nanoscience and Nanotechnology (2011) 11, 8054-8060
41. Masi, M.; Cavallotti, C.; Raffa, E. Modeling of flame assisted chemical vapor deposition of silicon films (2011) Crystal Research And Technology, vol. 46, p. 865-870
42. Dinon, F.; Salvalaglio, M.; Gallotta, A.; Beneduce, L.; Pengo, P.; Cavallotti, C.; Fassina, G. Structural refinement of protein A mimetic peptide (2011) Journal of Molecular Recognition, vol. 24, p. 1087-1094
43. Derudi, M.; Polino, D.; Cavallotti, C. Toluene and benzyl decomposition mechanisms: elementary reactions and kinetic simulations (2011) Physical Chemistry Chemical Physics, vol. 13, p. 21308-21318
44. Shukla, D.; Zamolo, L.; Cavallotti, C.; Trout, B.L. Understanding the Role of Arginine as an Eluent in Affinity Chromatography via Molecular Computations (2011) Journal of Physical Chemistry. B, vol. 115, p. 2645-2654
45. Salvalaglio, M.; Muscionico, I.; Cavallotti, C. Determination of Energies and Sites of Binding of PFOA and PFOS to Human Serum Albumin (2010) Journal of Physical Chemistry. B, vol. 114, p. 14860-14874
46. Cavallotti, C. Reactivity of Silicon Surfaces in the Presence of Adsorbed Hydrogen and Chlorine (2010) Chemical Vapor Deposition, vol. 16, p. 329-335, ISSN: 0948-1907
47. Polino, D.; Barbato, A.; Cavallotti, C. Theoretical investigation of germane and germylene decomposition kinetics (2010) Phys. Chem. Chem. Phys. 12, 10622.
48. Barbato, A.; Cavallotti, C. Challenges of introducing quantitative elementary reactions in multiscale models of thin film deposition Phys. Status Solidi B 2010, 247, 2127 (2010).
49. Zamolo, L.; Salvalaglio, M.; Cavallotti, C.; Galarza, B.; Sadler, C.; Williams, S.; Hofer, S.; Horak, J.; Lindner, W. Experimental and theoretical investigation of effect of spacer arm and support matrix of synthetic affinity chromatographic materials for the purification of monoclonal antibodies (2010) J. Phys. Chem. B, 2010, 114, 9367.
50. Salvalaglio, M.; Zamolo, L.; Busini, V.; Moscatelli, D.; Cavallotti, C. Molecular modeling of protein A affinity chromatography (2009) J. Chromatography A. 1216, 8678.

51. Boi, C.; Busini, V.; Salvalaglio, M.; Cavallotti, C.; Sarti, G.C. Understanding ligand–protein interactions in affinity membrane chromatography for antibody purification (2009) J. Chromatography A. 1286, 8687-8696.
52. Moiseev, T.; Isella, G.; Chrastina, D.; Cavallotti, C. Langmuir probe plasma parameters and kinetic rates in a Ar-SiH_4-H_2 plasma during nc-Si films deposition for photovoltaic applications (2009) J. Phys. D, 42, 225202.
53. Moiseev, T.; Chrastina, D.; Isella, G.; Cavallotti, C. Threshold ionization mass spectrometry in the presence of excited silane radicals (2009), J. Phys. D, 42, 072003.
54. Cavallotti, C.; Derudi, M.; Rota, R. On the mechanism of decomposition of the benzyl radical. (2009) Proc. Comb. Inst. 32, 115-121.
55. Barbato, A.; Seghi, C.; Cavallotti, C. An ab initio Rice-Ramsperger-Kassel-Marcus/master equation investigation of SiH_4 decomposition kinetics using a kinetic Monte Carlo approach (2009) J. Chem. Phys. 130 (7), 074108.
56. Novikov, P.L.; Le Donne, A.; Cereda, S.; Miglio, L.; Pizzini, S.; Binetti, S.; Rondanini, M.; Cavallotti, C.; Chrastina, D.; Moiseev, T.; von Känel, H.; Isella, G.; Montalenti, F. Phenomenological model of nanocrystalline silicon film formation by plasma-enhanced chemical vapor deposition (2009) Optoelectronics, Instrumentation and Data Processing 45 (4), 322-327.
57. Novikov, P.L.; Le Donne, A.; Cereda, S.; Miglio, L.; Pizzini, S.; Binetti, S.; Rondanini, M.; Cavallotti, C.; Chrastina, D.; Moiseev, T. von Kanel, H.; Isella, G.; Montalenti, F. Crystallinity and microstructure in Si films grown by plasma-enhanced chemical vapor deposition: A simple atomic-scale model validated by experiments (2009) Appl. Phys. Lett. 94 (5), 051904.
58. Moiani, D.; Salvalaglio, M.; Cavallotti, C.; Bujacz, A.; Redzynia, I.; Bujacz, G.; Dinon, F.; Pengo, P.; Fassina, G. Structural characterization of a Protein A mimetic peptide dendrimer bound to human IgG (2009) J. Phys. Chem. B 113, 16268-16275.
59. Cavallotti, C.; Metrangolo, P.; Meyer, F.; Recupero, F.; Resnati, G. Binding energies and 19F nuclear magnetic deshielding in paramagnetic halogen-bonded complexes of TEMPO with haloperfluorocarbons (2008) J. Phys. Chem. A 112 (40), 9911-9918.
60. Rondanini, M.; Cavallotti, C.; Ricci, D.; Chrastina, D.; Moiseev, T.; von Kanel, H.; Isella, G. An experimental and theoretical investigation of a magnetically confined dc plasma discharge (2008) J. Appl. Phys. 104, 013304.
61. Moiani, D.; Cavallotti, C.; Famulari, A.; Schmuck, C. Oxoanion binding by guanidiniocarbonylpyrrole cations in water: A combined DFT and MD investigation (2008) Chemistry A 14(17), 5207-5219.
62. Zamolo, L.; Busini, V; Moiani, D; Cavallotti, C. Molecular dynamic investigation of the interaction of supported affinity ligands with monoclonal antibodies (2008) Biotech. Prog. 24 (3), 527-539.
63. Moscatelli, D.; Dossi, M.; Cavallotti, C.; Storti, G.; Ab initio calculation of the propagation kinetics in free radical polymerization: Chain length and penultimate effects (2007) Macromolecular symposia 259 (1), 337-347.
64. Rondanini, M; Cereda, S; Montalenti, F; Miglio, L.; Cavallotti, C. A multiscale model of the plasma assisted deposition of crystalline silicon (2007) Surf. Coat. Tech. 201(22-23), 8863-8867.
65. Barbato, A; Fiorucci, A; Rondanini, M; Cavallotti, C.; Multiscale investigation of the influence of surface morphology on thin film CVD (2007) Surf. Coat. Tech. 201 (22-23): 8884-8887.
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67. Moscatelli, D; Cavallotti, C Theoretical investigation of the gas-phase kinetics active during the GaN MOVPE (2007) J. Phys. Chem. A, 111 (21): 4620-4631.

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