

LE PUBBLICAZIONI SCIENTIFICHE PRODOTTE CON IL CONTRIBUTO DEL CASPUR NEL TRIENNIO 2007-2009

a cura di Susana Bueno e Maria Pia Colapenna

2009

1. Abbate, I., Rozera, G., Bruselles, A., Vlassi, C., D'Offizi, G., Narciso, P., Chillemi, G., Prosperi, M., Ippolito, G. & Capobianchi, M. R. (2009). Dynamic variations of lymphocyte and monocyte-associated HIV-1 quasispecies after discontinuation of highly active anti-retroviral therapy as assessed by massively parallel pyrosequencing. *Infection*, **37**(S2), 22.
2. Ajmone Marsan, P., Marino, R., Perini, D., Negrini, R., Nicolazzi, E., Pariset, L., Valentini, A., Vicario, D., Santus, E., Blasi, M., Fontanesi, L., Schiavini, F., Bagnato, A., Maciotta, N. & Nardone, A. (2009). *Identification of selection signature across genome based on a 54,000 SNP panel*. 60th Annual meeting of the European Association for Animal Production.
3. Amati, F., Chillemi, G. & Novelli, G. (2009). *Gene expression analysis during development by high-throughput methods*. Nova Science Publishers.
4. Ayguade, E., Copty, N., Duran, A., Hoeflinger, J., Lin, Y., Massaioli, F., Teruel, X., Unnikrishnan, P. & Zhang, G. (2009). The design of openMP tasks. *IEEE T. Parall. Distr.*, **20**, 404-418.
5. Baccarelli, I., Sebastianelli, F., Gianturco, F. A. & Sanna, N. (2009). Modelling dissociative dynamics of biosystems after meta-stable electron attachment: the sugar backbones. *Eur. Phys. J. D*, **51**(1), 131-136.
6. Bailon-Cuba, J., Leonardi, S. & Castillo, L. (2009). Turbulent channel flow with 2D wedges of random height on one wall. *Int. J. Heat Fluid Fl.*, **30**(5), 1007-1015.
7. Baldazzi, V., Paci, P., Bernaschi, M. & Castiglione, F. (2009). Modeling lymphocyte homing and encounters in lymph nodes. *BMC Bioinformatics*, **10**(1), 387.
8. Bec, J., Biferale, L., Cencini, M., Lanotte, A. S. & Toschi, F. (2009). Caustics and intermittency in turbulent suspensions of heavy particles. *ArXiv e-prints arXiv:0905.1192v1 [physics.flu-dyn]*.
9. Bernardini, M., Orlandi, P., Pirozzoli, S. & Fabiani, F. (2009). *Statistics and flow structures in Couette-Poiseuille flows*. Progress in Wall Turbulence: Understanding and modeling, Lille, April 21-23.
10. Bernaschi, M., Melchionna, S., Succi, S., Fyta, M., Kaxiras, E. & Sircar, J. K. (2009). MUPHY: a parallel Multi PHYSics/scale code for high performance bio-fluidic simulations. *Comput. Phys. Commun.*, **180**(9), 1495-1502.
11. Berrone, S., Marro, M. & Garbero, V. (2009). Numerical simulation of low Reynolds number flows past rectangular cylinders based on adaptive finite element and finite volume methods. La Matematica e le sue Applicazioni, Pubblicazioni del Dipartimento di Matematica, Università di Torino, .
12. Bilanceri, M., Beux, F. & Salvetti, M. V. (2009). *Investigation on numerical schemes in the simulation of barotropic cavitating flows*. Proceedings of the 7th International Symposium on Cavitation.
13. Biocca, S., Falconi, M., Filesi, I., Baldini, F., Vecchione, L., Mango, R., Romeo, F., Federici, G., Desideri, A. & Novelli, G. (2009). Functional analysis and molecular dynamics simulation of LOX-1 K167N polymorphism reveal alteration of receptor activity. *PLoS One*, **4**(2), e4648.
14. Bocchinfuso, G., Mazzuca, C., Palleschi, A., Pizzoferrato, R. & Tagliatesta, P. (2009). Photophysical properties of 1,3,5-Tris(2-naphthyl)benzene and related less-arylated compounds: experimental and theoretical investigations. *J. Phys. Chem., A*, **113**(52), 14887-14895.
15. Bocchinfuso, G., Palleschi, A., Orion, B., Grande, G., Formaggio, F., Toniolo, C., Park, Y., Hahm, K. S. & Stella, L. (2009). Different mechanisms of action of antimicrobial peptides: insights from fluorescence spectroscopy experiments and molecular dynamics simulations. *J. Pept. Sci.*, **15**(9), 550-558.
16. Bodo, E. (2009). Low and ultra-low energy chemical processes involving ions. *Physica Scripta*, **80**, 048117-048122.

17. Bongiorni, S., Chillemi, G., Prosperini, G., Bueno, S., Signorelli, F., Moioli, B. & Pariset, L. (2009). Transcriptomic analysis of two sheep breeds during lactation, using a new custom microarray platform. *Ital. J. Anim. Sci.*, **8**, 33-35.
18. Bongiorni, S., Chillemi, G., Prosperini, G., Bueno, S., Valentini, A. & Pariset, L. (2009). *A tool for sheep product quality: custom microarray from public databases*. International Conference Foodomics.
19. Bongiorni, S., Chillemi, G., Prosperini, G., Bueno, S., Valentini, A. & Pariset, L. (2009). A tool for sheep product quality: custom microarrays from public databases. *Nutrients*, **1**, 235-250.
20. Bovino, S., Coccia, E., Bodo, E., Lopez-Duran, D. & Gianturco, F. A. (2009). Spin-driven structural effects in alkali doped ^4He clusters from quantum calculations. *J. Chem. Phys.*, **130**, 224903-224913.
21. Bovino, S., Wernli, M. & Gianturco, F. A. (2009). Fast LiH destruction in reaction with H: quantum calculations and astrophysical consequences. *Astrophys. J.*, **699**(1), 383-387.
22. Broglia, R., Bouscasse, B., Di Mascio, A., Lugni, C. & Atsavapranee, P. (2009). *Experimental and Numerical Analysis of the Roll Decay Motion for a Patrol Boat*. 19th International Offshore and Polar Engineers Conference, Osaka, Japan, June.
23. Broglia, R., Muscari, R. & Di Mascio, A. (2009). *Analysis of the roll decay motion for a patrol boat by URANS simulations*. OMAE 2009, 28th International Conference on Offshore Mechanics and Arctic Engineering, Honolulu, Hawaii, (USA), June.
24. Broglia, R., Zaghi, S. & Di Mascio, A. (2009). *Analysis of the hydrodynamic performances of high-speed catamarans by viscous flow solver*. 19th International Offshore and Polar Engineers Conference, Osaka, Japan, June.
25. Brzek, B., Bailon-Cuba, J., Leonardi, S. & Castillo, L. (2009). Theoretical evaluation of the Reynolds shear stress and flow parameters in transitionally rough turbulent boundary Layers. *J. Turbul.*, **10**, N5.
26. Caliandro, R., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Mazzone, A. M. & Siliqi, D. (2009). EDM-DEDM and protein crystal structure solution. *Acta Cryst.*, **65**, 477-484.
27. Capitani, G. C., Stixrude, L. & Mellini, M. (2009). First-principles energetics and structural relaxation of antigorite. *Am. Mineral.*, **94**(8-9), 1271-1278.
28. Ceccarelli, M. (2009). Simulating transport properties through bacterial channels. *Frontiers in Bioscience*, **14**, 3222-3238.
29. Chiani, F., Iannone, C., Negri, R., Paoletti, D., D'Antonio, M. R., D'Onorio De Meo, P. & Castrignanò, T. (2009). Radiation Genes: a database devoted to microarrays screenings revealing transcriptome alterations induced by ionizing radiation in mammalian cells. *Database*, **2009**(0), bap007.
30. Chillemi, G., Coletta, A., Mancini, G., Sanna, N. & Desideri, A. (2009). An amber compatible molecular mechanics force field for the anticancer drug topotecan. *Theor. Chem. Acc.*
31. Chinappi, M. & Casciola, C. M. (2009). *Intrinsic slip on hydrophobic surfaces*. AIMETA 2009, Associazione Italiana di Meccanica Teorica e Applicata, Ancona, 14-17 Settembre.
32. Ciccioli, A., Gigli, G. & Meloni, G. (2009). The Si-Sn Chemical Bond: An Integrated Thermochemical and Quantum Mechanical Study of the SiSn Diatomic Molecule and Small Si-Sn Clusters. *Chem-Eur. J.*, **15**(37), 9543-9560.
33. Coccia, E., Bodo, E. & Gianturco, F. A. (2009). Size-dependent solvation of p-H₂ in ^4He : A quantum Monte Carlo analysis. *J. Chem. Phys.*, **130**, 094906-094910.
34. Colizzi, G., Biddau, G. & Fiorentini, V. (2009). Indium on Cu(100) from first principles: Energetics, complex formation, and diffusion of adsorbates and vacancies on terraces and at steps. *Phys. Rev. B*, **79**(16), 165441.
35. Colizzi, G., Filippetti, A., Cossu, F. & Fiorentini, V. (2009). Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO₃. *Eur. Phys. J. B*, **70**(3), 343-346.
36. Collu, F., Spiga, E., Kumar, A., Hajjar, E., V, V. A., Ceccarelli, M. & Ruggerone, P. (2009). Drug Design: Insights from atomistic simulations. *Nuovo Cimento C*, **32**(2), 67-71.
37. Cristiani, E. & Falcone, M. (2009). Fully-discrete schemes for the value function of Pursuit-Evasion games with state constraints. *Annals of Dynamic Games*, **10**, 178-205.
38. D'Abramo, M., Caminiti, R., Di Nola, A. & Amadei, A. (2009). What can we learn by comparing experimental and theoretical-computational X-ray scattering data? *J. Mol. Liq.*, **144**(1-2), 9-12.
39. D'Abramo, M., Di Nola, A. & Amadei, A. (2009). Kinetics of Carbon Monoxide Migration and Binding in Solvated Myoglobin as Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. *J. Phys. Chem. B*, **113**(51), 16346-16353.
40. D'Andria, P., Viggiano, A. & Magi, V. (2009). *On the Performance of a Compressible LES Parallel Code for the Simulation of Transient Jets*. Libreria Universitaria Benedetti, L'Aquila.
41. D'Angelo, P., Zitolo, A., Migliorati, V., Mancini, G., Persson, I. & Chillemi, G. (2009). Structural investigation of lanthanoid coordination: a combined XANES and molecular dynamics study. *Inorg. Chem.*, **48**(21), 10239-10248.
42. D'Annessa, I., Chillemi, G. & Desideri, A. (2009). Structural-dynamical properties of the Deinococcus radiodurans topoisomerase IB in absence of DNA: correlation with the human enzyme. *J. Biomol. Struct. Dyn.*, **27**(3), 307-318.
43. D'Antonio, M., Castrignanò, T., Mignone, F., Chillemi, G., Mancini, G., Valentini, A. & Pesole, G. (2009). *Genome wide analysis of the alternative splicing pattern in cow*. XVIII Congresso Aspa, Palermo 2009.

44. De Petris, G., Festa, M. R., Galantini, L., Giglio, E., Leggio, C., Pavel, N. V. & Troiani, A. (2009). Sodium Glycodeoxycholate and Glycocholate Mixed Aggregates in Gas and Solution Phases. *J. Phys. Chem. B*, **113**(20), 7162-7169.
45. De Tullio, M. D., Cristallo, A., Balaras, E. & Verzicco, R. (2009). Direct numerical simulation of the pulsatile flow through an aortic bileaflet mechanical heart valve. *J. Fluid. Mech.*, **622**(-1), 259-290.
46. Debernardi, A. & Fanciulli, M. (2009). Ab initio study of the magnetic interaction of Co and Ni doped ZnO with intrinsic vacancies. *Physica B: Condensed Matter*, **404**(23-24), 4791-4793.
47. Delugas, P., Fiorentini, V. & Filippetti, A. (2009). Dielectric and vibrational properties of bixbyite sesquioxides. *Phys. Rev. B*, **80**(10), 104301.
48. Falcone, M. & Rorro, M. (2009). *On the computation of the effective Hamiltonian in the nonconvex case*. APSCT'2009, Actual Problems of Stability and Control Theory. Institute of Mathematics and Mechanics of the Ural Branch of the Russian Academy of Sciences, Ural State University, Ekaterinburg, Russia, September 21-26.
49. Falcone, M. & Rorro, M. (2009). *Optimization techniques for the computation of the effective Hamiltonian*. BFG'09 Recent Advances in Optimization and its Applications in Engineering, Leuven, September 14-18.
50. Falconi, M., Oteri, F., Chillemi, G., Andersen, F. F., Tordrup, D., Oliveira, C. L. P., Pedersen, J. S., Knudsen, B. R. & Desideri, A. (2009). Deciphering the Structural Properties That Confer Stability to a DNA Nanocage. *ACS Nano*, **3**(7), 1813-1822.
51. Filippetti, A. & Fiorentini, V. (2009). A practical first-principles band-theory approach to the study of correlated materials. *Eur. Phys. J. B*, **71**(2), 139-183.
52. Filippetti, A., Puggioni, D. & Fiorentini, V. (2009). Fermi-surface pockets in magnetic underdoped cuprates from first principles. *Europhys Lett.*, **88**(6), 67009.
53. Finelli, I., Chiessi, E., Galessio, D., Renier, D. & Paradossi, G. (2009). Gel-like structure of a hexadecyl derivative of hyaluronic acid for the treatment of osteoarthritis. *Macromol. Biosci.*, **9**(7), 646-653.
54. Fiorani, P., Tesauro, C., Mancini, G., Chillemi, G., D'Annessa, I., Graziani, G., Tentori, L., Muzi, A. & Desideri, A. (2009). Evidence of the crucial role of the linker domain on the catalytic activity of human topoisomerase I by experimental and simulative characterization of the Lys681Ala mutant. *Nucleic Acids Res.*, **37**(20), 6849-6858.
55. Franz, J., Baccarelli, I., Caprasecca, S. & Gianturco, F. A. (2009). Computed vibrational excitation of CF_4 by low-energy electrons and positrons: comparing calculations and experiments. *Phys. Rev. A*, **80**(1), 012709.
56. Gentilini, S., Fratalocchi, A., Angelani, L., Ruocco, G. & Conti, C. (2009). Ultrashort pulse propagation and the Anderson localization. *Opt. Lett.*, **34**(2), 130-132.
57. Ghio, C., Lazzaroni, R. & Alagona, G. (2009). Computational results provide a synthetically unprecedented explanation for the beta-regioselectivity in the rh-catalyzed hydroformylation of vinylidene substrates. *Eur. J. Inorg. Chem.*, **2009**(1), 98-103.
58. Gianturco, F. A. & Tacconi, M. (2009). Concluding remarks: achievements and challenges in cold and ultracold molecules. *Faraday Discuss.*, **142**, 463-477.
59. González, E. M., Guidoni, L. & Molteni, C. (2009). Chemical and protein shifts in the spectrum of the photoactive yellow protein: a time-dependent density functional theory/molecular mechanics study. *Phys. Chem. Chem. Phys.*, **11**, 4556-4563.
60. Gori, P., Contini, G., Prosperi, T., Ronci, F., Colonna, S., Zema, N., Turchini, S., Catone, D., Criscenti, A. & Palma, A. (2009). Adsorption and self-assembly of D-alaninol on Cu(100). *Superlattices and Microstructures*, **46**(1-2), 52-58.
61. Goumans, T. P. M., Gianturco, F. A., Sebastianelli, F., Baccarelli, I. & Rivail, J. L. (2009). Dissociative Electron Attachment to Formamide: Direct and Indirect Pathways from Resonant Intermediates. *J. Chem. Theory Comput.*, **5**(1), 217-221.
62. Grottesi, A., Mancini, G., Desideri, A. & Chillemi, G. (2009). Molecular modelling of BCRP (ABCG2) multidrug resistance protein and docking of new camptothecin analogues. *Biophys. J.*, **96**(3, Supplement 1), 599a.
63. Guidoni, L., Gontrani, L., Bencivenni, L., Sadun, C. & Ballirano, P. (2009). Overcoming the inadequacy of x-ray powder diffraction in reliable hydrogen location with the aid of first principles calculations: crystal structure determination of orotaldehyde monohydrate. *J. Phys. Chem. A*, **113**(1), 353-359.
64. Horner, D. S., Pavesi, G., Castrignanò, T., D'Onorio De Meo, P., Liuni, S., Sammeth, M., Picardi, E. & Pesole, G. (2009). Bioinformatics approaches for genomics and post genomics applications of next-generation sequencing. *Brief. Bioinform.*, bbp046.
65. Iemma, U. & Burghignoli, L. (2009). *A hermite-coons boundary element method*. 16th International Congress on Sound and Vibration, ICSV16, Krakow, Poland, July.
66. Iemma, U., Marchese, V. & Gori, R. (2009). *AcouSTO - a new open-source project for acoustic simulation*. 16th International Congress on Sound and Vibration, ICSV16, Krakow, Poland, July.
67. Lopez-Duran, D., Tacconi, M. & Gianturco, F. A. (2009). $\text{LiH} - (\text{C}^2\text{S}^+)$ + $^{3,4}\text{He}$ rotational quenching at ultralow energies: spin-flip and isotopic effects from quantum dynamics on an ionic system. *Eur. Phys. J. D*, **55**(3), 601-611.
68. Lotito, L., Russo, A., Bueno, S., Chillemi, G., Fogli, M. V. & Capranico, G. (2009). A specific transcriptional response of yeast cells to camptothecin dependent on the Swi4 and Mbp1 factors. *Eur. J. Pharmacol.*, **603**(1-3), 29-36.

69. Marquez-Mijares, M., Perez de Tudela, R., Gonzalez-Lezana, T., Roncero, O., Miret-Artes, S., Delgado-Barrio, G., Villarreal, P., Baccarelli, I., Gianturco, F. A. & Rubayo-Soneira, J. (2009). A theoretical investigation on the spectrum of the Ar trimer for high rotational excitations. *J. Chem. Phys.*, **130**(15).
70. Migliorati, V., Chillemi, G., Mancini, G., Zitolo, A., Tatoli, S., Filippini, A. & D'Angelo, P. (2009). Ion hydration in high-density water. *J. Phys.: Conf. Ser.*, **190**(012057).
71. Murgiano, L., Timperio, A. M., D'Amici, G. M., Pariset, L., Valentini, A. & Zolla, L. (2009). *Proteomic study: liver metabolism through a comparison of the protein expression profiles of the two breeds Chianina and Holstein*. IV International Symposium Of Livestock Production.
72. Orioni, B., Bocchinfuso, G., Kim, J. Y., Palleschi, A., Grande, G., Bobone, S., Park, Y., Kim, J. I., Hahm, K. S. & Stella, L. (2009). Membrane perturbation by the antimicrobial peptide PMAP-23: a fluorescence and molecular dynamics study. *Biochimica Et Biophysica Acta-biomembranes* **1788**(7), 1523-1533.
73. Orlandi, P. (2009). Energy spectra power laws and structures. *J. Fluid Mech.* **623**, 353-374.
74. Orlandi, P. (2009). Rough channels, *in* TSFP-6: turbulence and shear flow phenomena. Seoul National University, Seoul, Korea, June 22-24.
75. Orlandini, S., Baccarelli, I. & Gianturco, F. A. (2009). Variational calculations of structures and energetics in very floppy trimers: A new computational implementation. *Comput. Phys. Commun.*, **180**(3), 384-391.
76. Paci, P., Carello, R., Bernaschi, M., D'Offizi, G. & Castiglione, F. (2009). Immune control of HIV-1 infection after therapy interruption: immediate versus deferred antiretroviral therapy. *BMC Infectious Diseases*, **9**(1), 172.
77. Paparella, F. & Von Hardenberg, J. (2009). *On the statistics of scalar fluctuations in fingering convection*. Proceedings "WASCOM 2009" 15th conference on Waves and Stability in Continuous Media, World Scientific, 315-320.
78. Pariset, L., Caroli, A., Chessa, S., Fontanesi, L., Russo, V., Bagnato, A., Schiavini, F., Samorè, A. B., Feligini, M., Bonizzi, I., Vicario, D., Rossoni, A., Sangalli, S., Marino, R., Perini, D., Nicolazzi, E., Macciotta, N. & Ajmone Marsan, P. (2009). Assessment of 29 candidate genes for milk traits in Italian dairy cattle. *Ital. J. Anim. Sci.*, **8**(supp.2), 226.
79. Pariset, L., Chillemi, G., Bongiorni, S., Spica, V. R. & Valentini, A. (2009). Microarrays and high-throughput transcriptomic analysis in species with incomplete availability of genomic sequences. *N. Biotechnol.*, **25**(5), 272-279.
80. Pariset, L., Chillemi, G., Bueno, S., Prosperini, G., Bongiorni, S., Moioli, B. & Valentini, A. (2009). *Transcriptomic analysis for species without annotated genomic dna sequences*. Plant & Animal Genomes XVII Conference.
81. Peralta, G., Puggioni, D., Filippetti, A. & Fiorentini, V. (2009). Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. *Phys. Rev. B*, **80**(14), 140408.
82. Pica Ciamarra, M. & Coniglio, A. (2009). Jamming at Zero Temperature, Zero Friction, and Finite Applied Shear Stress. *Phys. Rev. Lett.*, **103**(23), 235701.
83. Pirozzoli, S. (2009). *On the relationship between vortex sheets and tubes in wall-bounded flows*. Progress in Wall Turbulence: understanding and modeling, Lille, April 21-23.
84. Pirozzoli, S., Beer, A., Bernardini, M. & Grasso, F. (2009). Computational analysis of impinging shock-wave boundary layer interaction under conditions of incipient separation. *Shock Waves*, **19**(6), 487-497.
85. Ponzi, A., Marinetti, F. & Gianturco, F. A. (2009). Structuring molecular hydrogen around ionic dopants: Li⁺ cations in small pH(2) clusters. *Phys. Chem. Chem. Phys.*, **11**(20), 3868-3874.
86. Prosmiti, R., Delgado-Barrio, G., Villarreal, P., Yurtsever, E., Coccia, E. & Gianturco, F. A. (2009). Structuring a Quantum Solvent around a Weakly Bound Dopant: The He-CS₂(³S₀) Complex. *J. Phys. Chem. A*, **113**(52), 14718-14729.
87. Prosperini, G., Bueno, S., Mancini, G., Chillemi, G., Pariset, L. & Valentini, A. (2009). *How transcriptomic reflects selection for milk and meat traits: kegg pathways and gene ontology in two cattle breeds*. International Conference Foodomics.
88. Puggioni, D., Filippetti, A. & Fiorentini, V. (2009). Fermi-surface pockets in YBa₂Cu₃O_{6.5}: comparison of ab initio techniques. *Phys. Rev. B*, **79**(6), 064519.
89. Ramondo, F., Tanzi, L., Campetella, M., Gontrani, L., Mancini, G., Pieretti, A. & Sadun, C. (2009). Hydration of diazoles in water solution: pyrazole. A theoretical and X-ray diffraction study. *Phys. Chem. Chem. Phys.*, **11**, 9431-9439.
90. Robertazzi, A., Vargiu, A. V., Magistrato, A., Ruggerone, P., Carloni, P., De Hoog, P. & Reedijk, J. (2009). Copper-1,10-Phenanthroline complexes binding to DNA: structural predictions from molecular simulations. *J. Phys. Chem. B*, **113**(31), 10881-10890.
91. Roman, F., Armenio, V. & Froehlich, J. (2009). A simple wall-layer model for large eddy simulation with immersed boundary method. *Phys. Fluids*, **21**(10), 101701.
92. Rozera, G., Abbate, I., Bruselles, A., Vlassi, C., D'Offizi, G., Narciso, P., Chillemi, G., Prosperi, M., Ippolito, G. & Capobianchi, M. R. (2009). Massively parallel pyrosequencing highlights minority variants in the HIV-1 env quasispecies deriving from lymphomonocyte sub-populations. *Retrovirology*, **6**, 15.
93. Rozera, G., Abbate, I., Bruselles, A., Vlassi, C., D'Offizi, G., Narciso, P., Chillemi, G., Prosperi, M., Ippolito, G. & Capobianchi, M. R. (2009). Archived HIV-1 minority variants detected by ultra-deep pyrosequencing in provirus may be fully replication competent. *AIDS*, **23**(18), 2541-2543.

- 94.** Rutigliano, M., Zazza, C., Sanna, N., Mancini, G., Barone, V., Aschi, M. & Caciatore, M. (2009). Oxygen adsorption on beta cristobalite polymorph: ab-initio modeling and semi-classical Time-dependent dynamics. *J. Phys. Chem. A*, **113**, 15366-15375.
- 95.** Sanchez-Roman, A., Sannino, G., Garcia-Lafuente, J., Carillo, A. & Criado-Aldeanueva, F. (2009). Transport estimates at the western section of the Strait of Gibraltar: a combined experimental and numerical modeling study. *J. Geophys. Res.*, **114**(C6), C06002.
- 96.** Sanna, N., Baccarelli, I. & Morelli, G. (2009). SCELib3.0: the new revision of SCELib, the parallel computational library of molecular properties in the single center approach. *Comput. Phys. Commun.*, **180**(12), 2544-2549.
- 97.** Sanna, N., Baccarelli, I. & Morelli, G. (2009). The VOLSCAT package for electron and positron scattering of molecular targets: A new high throughput approach to cross-section and resonances computation. *Comput. Phys. Commun.*, **180**(12), 2550-2562.
- 98.** Sanna, N., Chillemi, G., Gontrani, L., Grandi, A., Mancini, G., Castelli, S., Zagotto, G., Zazza, C., Barone, V. & Desideri, A. (2009). UV-vis spectra of the anticancer camptothecin family drugs in aqueous solution: specific spectroscopic signatures unraveled by a combined computational and experimental study. *J. Phys. Chem. B*, **113**(16), 5369-5375.
- 99.** Sannino, G., Herrmann, M., Carillo, A., Rupolo, V., Ruggiero, V., Artale, V. & Heimbach, P. (2009). An eddy-permitting model of the Mediterranean sea with a two-way grid refinement at the Strait of Gibraltar. *Ocean Modelling* **30**(1), 56-72.
- 100.** Sannino, G., Pratt, L. & Carillo, A. (2009). Hydraulic criticality of the exchange flow through the Strait of Gibraltar. *J. Phys. Oceanogr.*, **39**(11), 2779-2799.
- 101.** Scorciapino, A. M., Robertazzi, A., Casu, M., Ruggerone, P. & Ceccarelli, M. (2009). Breathing motions of a respiratory protein revealed by molecular dynamics simulations. *J. Am. Chem. Soc.*, **131**, 11825-11832.
- 102.** Sebastianelli, F., Gianturco, F. A., Stoecklin, T. & Baccarelli, I. (2009). Scattering of electrons by gaseous CS(¹S): The role of short-range forces on the very-low energy ²P resonance. *Chem. Phys. Lett.*, **476**(4-6), 182-185.
- 103.** Tacconi, M. & Gianturco, F. A. (2009). Exchanging the ionic partner in a linear Paul trap: the MgH⁺(X ¹S⁺) ion with neutral Rb(S-2). *Eur. Phys. J. D*, **54**(1), 31-41.
- 104.** Tacconi, M. & Gianturco, F. A. (2009). Translational cooling versus vibrational quenching in ultracold OH-Rb collisions: a quantum assessment. *J. Chem. Phys.*, **131**(9).
- 105.** Tai, K., Haider, S., Grottesi, A. & Sansom, M. S. P. (2009). Ion channel gates: comparative analysis of energy barriers. *Eur. Biophys. J.*, **38**(4), 347-354.
- 106.** Tatoli, S., Zazza, C., Sanna, N., Palma, A. & Aschi, M. (2009). The role of Arginine 38 in horseradish peroxidase enzyme revisited: a computational investigation. *Biophys. Chem.*, **141**(1), 87-93.
- 107.** Timperio, A. M., D'Alessandro, A., Pariset, L., D'Amici, G. M. & Zolla, L. (2009). Comparative proteomics and transcriptomics analyses of livers from two different Bos taurus breeds: "Chianina and Holstein Friesian". *Journal of Proteomics*, **73**, 309-322.
- 108.** Tordella, D. & Iovieno, M. (2009). Decay exponent of large and small scales in isotropic turbulence. Proceedings of EUROMECH Colloquium 512. Small Scale turbulence and related gradient statistics. Classe di Scienze Fisiche, Matematiche e Naturali, suppl.2009, **142**, 128-129.
- 109.** Tordella, D. & Iovieno, M. (2009). Small scale anisotropy induced by a spatial variation of the integral scale. Proceedings of EUROMECH Colloquium 512. Small Scale turbulence and related gradient statistics. Atti della Accademia delle Scienze di Torino. Classe di Scienze Fisiche, Matematiche e Naturali, suppl.2009, **142**, 108-111.
- 110.** Valentini, A., Pariset, L., Bongiorni, S., D'Andrea, M. S., Pilla, F., Guarini, R., Filippini, F., Williams, J. L., Ajmone Marsan, P. & Nardone, A. (2009). Preliminary results of a genome scan of Marchigiana cattle typed by a Illumina 54,000 SNP panel. 60th Annual meeting of the European Association for Animal Production.
- 111.** Valentini, A., Pariset, L., Bongiorni, S., Williams, J. L., Ajmone Marsan, P., D'Andrea, M. S., Pilla, F., Quaglino, A., Albera, A. & Nardone, A. (2009). A Signature of selection around the myostatin locus in Piedmontese cattle typed by a 54,000 SNP panel. 60th Annual meeting of the European Association for Animal Production.
- 112.** Venanzi, M., Bocchinfuso, G., Gatto, E., Palleschi, A., Stella, L., Formaggio, F. & Toniolo, C. (2009). Metal binding properties of fluorescent analogues of trichogin GA IV: a conformational study by time-resolved spectroscopy and molecular mechanics investigations. *ChemBioChem*, **10**(1), 91-97.
- 113.** Venanzi, M., Gatto, E., Bocchinfuso, G., Palleschi, A., Stella, L., Baldini, C., Formaggio, F., Toniolo, C. & Pispisa, B. (2009). Monitoring peptide folding by time-resolved spectroscopies: the effect of a single gly to aib substitution. *Peptides For Youth - the Proceedings of the 20th American Peptide Symposium*, **611**, 47-48.
- 114.** Venanzi, M., Gatto, E., Stella, L., Bocchinfuso, G., Palleschi, A., Formaggio, F. & Toniolo, C. (2009). Antimicrobial peptides chelating lanthanide ions: the case of trichogin GA IV analogues and terbium(III). *Peptides For Youth - the Proceedings of the 20th American Peptide Symposium*, **611**, 43-44.
- 115.** Vitagliano, L., Stanzione, F., Simone, A. D. & Esposito, L. (2009). Dynamics and stability of amyloid-like steric zipper assemblies with hydrophobic dry interfaces. *Biopolymers*, **91**(12), 1161-1171.

- 116.** Volodin, E. M., Diansky, N. A., Purini, R. & Transerici, C. (2009). *On the mechanism of natural variability of Atlantic Meridional Overturning Circulation in climate model.* INMCM3.0. Geophysical Research Abstracts, **11**, EGU2009-4133, 2009, EGU General Assembly.
- 117.** Volodin, E. M., Diansky, N. A., Purini, R. & Transerici, C. (2009). *On the variability of the Atlantic Meridional Overturning Circulation (AMOC) as resulting from the Global Climate Model.* INMCM3.0. Convegno S.I.F. Bari, 28 Settembre - 3 Ottobre 2009.
- 118.** Wernli, M., Caruso, D., Bodo, E. & Gianturco, F. A. (2009). Computing a three-dimensional electronic energy manifold for the LiH + H → Li + H₂ chemical reaction. *J. Phys. Chem. A*, **113**(6), 1121-1128.
- 119.** Wernli, M., Scifoni, E., Bodo, E. & Gianturco, F. A. (2009). A quantum modeling of the chemistry of LiH with He from ab initio calculations: ionic reactions in He nanodroplets. *Int. J. Mass Spectrom.*, **280**, 57-60.
- 120.** Zaghi, S., Broglia, R. & Di Mascio, A. (2009). *Experimental and numerical investigations on fast catamarans interference effects.* 9th International Conference on Hydrodynamics, Shanghai, China, October 11-15, 2010.
- 121.** Zanetti-Polzi, L., Anselmi, M., D'Alessandro, M., Amadei, A. & Di Nola, A. (2009). Structural, thermodynamic, and kinetic properties of gramicidin analogue GS6 studied by molecular dynamics simulations and statistical mechanics. *Biopolymers*, **91**(12, Sp. Iss. SI), 1154-1160.
- 122.** Zazza, C., Mancini, G., Sanna, N. & Aschi, M. (2009). In Silico characterization of a fourfold magnesium organometallic compound in PTCDA thin films. *J. Phys. Chem. A*, **113**, 14813-14817.
- 123.** Zazza, C., Mancini, G., Sanna, N. & Aschi, M. (2009). Thermodynamic features and environmental effects in a two-states molecular device under strict electrochemical control. *Theor. Chem. Acc.*, **123**, 383-390.
- 124.** Zhang, P., Bodo, E. & Dalgarno, A. (2009). Near resonance charge exchange in ion-atom collisions of lithium isotopes. *J. Phys. Chem. A*, **113**, 15085-15090.

2008

- 125.** Alcaro, S., Gontrani, L., Incani, O., & Ortuso, F. (2008). Computational methods applied to the discovery of stem cell factor ligands. *Theor. Chem. Acc.*, **120**, 523-531.
- 126.** Alesii, G. (2008). *Assessing least squares monte carlo for the kulatilaka trigeorgis general real options pricing model.* 43rd Euro Working Group on Financial Modelling, September 2008, London, UK.
- 127.** Amadei, A., Aschi, M., & Di Nola, A. (2008). *Statistical mechanical modeling of chemical reactions in condensed phase systems.* (Vol. 6) Springer.
- 128.** Amati, F., Giallonardi, S., Cipollone, D., Bueno, S., Vecchione, L., Prosperini, G., Desideri, A., Chillemi, G., Marino, B. & Novelli, G. (2008). *Genome-wide transcriptome profiling of mouse embryos with cardiac and thymic defects induced by an antagonist of retinoic acid.* Bi-Annual Meeting of the Working Group on Developmental Anatomy and Pathology, Alberobello (Bari), 12-15 march.
- 129.** Ambrogi, M. M. (2008). Simulazione del flusso attorno ad un bulbo di un'imbarcazione classe Coppa America. Tesi di Laurea in Ingegneria Aerospaziale.
- 130.** Ambrogi, M. M., Broglia, R., & Di Mascio, A. (2008). *Numerical simulation of a flow around an america's cup class keel.* 18th International Offshore and Polar Engineers Conference, July 2008, Vancouver (Canada).
- 131.** Aninati, F., Berettoni, M., Bigioni, M., Binaschi, M., Felicetti, P., Gontrani, L., et al. (2008). Synthesis, biological evaluation and molecular modeling studies of rebeccamycin analogues modified in the carbohydrate moiety. *Chem. Med. Chem.*, **3**, 266-279.
- 132.** Anselmi, M., Brunori, M., Vallone, B., & Di Nola, A. (2008). Molecular dynamics simulation of the euroglobin crystal: comparison with the simulation in solution. *Biophys. J.*, **95**(9), 4157-4162.
- 133.** Anselmi, M., Di Nola, A., & Amadei, A. (2008). The kinetics of ligand migration in crystallized myoglobin as revealed by molecular dynamics simulations. *Biophys. J.*, **94**(11), 4277-4281.
- 134.** Apollonio, F., Liberti, M., Amadei, A., Aschi, M., Pellegrino, M., D'Alessandro, M., et al. (2008). Mixed quantum-classical methods for molecular simulations of biochemical reactions with microwave fields: the case study of myoglobin. *IEEE T. Microw. Theory*, **56**(11), 2511-2519.
- 135.** Araya, G., Leonardi, S., & Castillo, L. (2008). Numerical assessment of local forcing on the heat transfer in a turbulent channel flow. *Phys. Fluids*, **20**(8), 085105.
- 136.** Arcovito, A., Moschetti, T., D'Angelo, P., Mancini, G., Vallone, B., Brunori, M., & Della Longa, S. (2008). An x-ray diffraction and x-ray absorption spectroscopy joint study of neuroglobin. *Arch. Biochem. Biophys.*, **475**, 7-13.
- 137.** Aschi, M., D'Alessandro, M., Pellegrino, M., Di Nola, A., D'Abromo, M., & Amadei, A. (2008). Intramolecular charge transfer in pi-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state. *Theor. Chem. Acc.*, **119**(5-6), 469-476.
- 138.** Ayguadé, E., Copty, N., Duran, A., Hoeflinger, J., Lin, Y., Massaioli, F., et al. (2008). *A proposal for task parallelism in openmp* (Vol. 4935) Springer Berlin-Heidelberg.

- 139.** Ayguadé, E., Duran, A., Hoeflinger, J., Massaioli, F., & Teruel, X. (2008). *An experimental evaluation of the new openmp tasking model* (Vol. 5234) Springer Berlin-Heidelberg.
- 140.** Baccarelli, I., Gianturco, F. A., Grandi, A., & Sanna, N. (2008). Metastable anion fragmentations after resonant attachment: deoxyribosic structures from quantum electron dynamics. *Int. J. Quantum Chem.*, **108**(11), 1878-1887.
- 141.** Baccarelli, I., Sanna, N., Gianturco, F. A., & Sebastianelli, F. (2008). Molecular mechanisms for electron-induced damage to biocomponents: cross sections and temporary anionic states for monosaccharides. *J. Phys.: Conf. Ser.*, **115**, 012009.
- 142.** Balducci, G., Brutti, S., Ciccioli, A., Trionfetti, G., Palenzona, A. & Pani, M. (2008). Thermodynamic properties of barium silicides from vapor pressure measurements and density functional calculations. *Intermetallics*, **16**(8), 1006-1012.
- 143.** Basher, S., & Fachin, S. (2008). The long-term decline of internal migration in canada: the case of ontario. *Lett. Spat. Resour. Sci.*, **1**, 171-181.
- 144.** Benzi, R. & Verzicco, R. (2008). Numerical simulations of flow reversal in Rayleigh-Bénard convection. *Europhys. Lett.*, **81**(6), 64008.
- 145.** Bersani, A. M., Carlini, E., Lanucara, P., Rorro, M., & Ruggiero, V. (2008). Application of optimal control techniques and advances computing to the study of enzyme kinetics. *Mathematics and Computers in Simulation (MATCOM)*, in press.
- 146.** Biczysko, M., Bloino, J., Pavone, M., Crescenzi, O., & Barone, V. (2008). *Approcci computazionali integrati per simulazioni di processi molecolari. Sviluppi ed applicazioni per lo studio di sistemi molecolari di interesse biologico*. Italian e-Science 2008, Università degli Studi di Napoli Federico II, Napoli, 27-29 Maggio 2008.
- 147.** Bloino, J., Biczysko, M., Crescenzi, O., & Barone, V. (2008). Integrated computational approach to vibrationally resolved electronic spectra: anisole as a test case. *J. Chem. Phys.*, **128**(24), 244105.
- 148.** Bocchinfuso, G. (2008). *Determination of antimicrobial peptide location inside lipid bilayers by combined fluorescence spectroscopy and md simulations*. 11th Naples Workshop on Bioactive Peptides, Naples, May, 2008.
- 149.** Bocchinfuso, G. (2008). *Determination of peptide location inside a lipid bilayer by combined fluorescence spectroscopy and molecular dynamics simulations. the case of the antimicrobial peptide pmap-23*. Acta Biophysica Romana 2008, Rome, April, 2008.
- 150.** Bocchinfuso, G. (2008). *Simulations of antimicrobial peptides : two case studies*. 1st Italy-Korea Symposium on Antimicrobial Peptides (8th RCPM International Symposium). Seosuk Hall, Chosun University, Gwangju, Korea July 24-25, 2008.
- 151.** Bocchinfuso, G., Mazzuca, C., Saracini, C., Venanzi, M., Micheli, L., Palleschi, G. & Palleschi, A. (2008). Receptors for organochlorine pesticides based on calixarenes. *Microchimica Acta*, **163**(3-4), 195-202.
- 152.** Bocchinfuso, G., Palleschi, A., Mazzuca, C., Coviello, T., Alhaique, F. & Marletta, G. (2008). Theoretical and experimental study on a self-assembling polysaccharide forming nanochannels: static and dynamic effects induced by a soft confinement. *J. Phys. Chem. B*, **112**(20), 6473-6483.
- 153.** Bodo, E., Zhang, P. & Dalgarno, A. (2008). Ultra-cold ion-atom collisions: near resonant charge exchange. *New J. Phys.*, **10**(3), 033024.
- 154.** Botti, M., Gonnella, G., Lamura, A., Massaioli, F., & Sofonea, V. (2008). A parallel thermal lattice boltzmann model with flux limiters for microscale flow. *Int. J. Mod. Phys. C*, **19**(12), 1847-1861.
- 155.** Bovino, S., Bodo, E., & Gianturco, F. A. (2008). Ultralow-energy vibrational quenching in ionic collisions: isotope effects in Li⁺ + d₂ encounters. *Phys. Rev. A*, **77**(4), 042716.
- 156.** Bovino, S., Bodo, E., Yurtsever, E., & Gianturco, F. A. (2008). Vibrational cooling of spin-stretched dimer states by He buffer gas: quantum calculations for Li-2(a(3)sigma(+))(u) at ultralow energies. *J. Chem. Phys.*, **128**(22), 224312.
- 157.** Brancato, G., Rega, N., Crescenzi, O., & Barone, V. (2008). *Un approccio computazionale integrato per la modellizzazione di sistemi molecolari complessi in soluzione*. Italian e-Science 2008, Università degli Studi di Napoli Federico II, Napoli, 27-29 Maggio 2008.
- 158.** Broglia, R., Di Mascio, A., & Muscari, R. (2008). *Numerical simulation of the roll decay motion for the "bettica" model ship, 6dof-ranse-ii/mou* (No. INSEAN TR 2008-046). INSEAN.
- 159.** Broglia, R., Muscari, R., & Di Mascio, A. (2008). *Numerical simulations of the pure sway and pure yaw motion of the kvlcc-1 and 2 tankers*. SIMMAN 2008, Workshop on Verification and Validation of Ship Manoeuvering Simulation Methods, April 14-16, Copenhagen (DK).
- 160.** Broglia, R., Di Mascio, A., & Amati, G. (2008). *Parallel unsteady rans code for the numerical simulations of free surface flows*. 9th SIMAI 2008, Rome (IT), September 15-19, 2008.
- 170.** Broglia, R., & Di Mascio, A. (2008). *Scale effect analysis and hydrodynamic performance of high-speed catamarans*. 27th ONR Symposium on Naval Hydrodynamics, October 5-10, 2008, Seoul, Korea.
- 171.** Broglia, R. (2008). *Task n5.in4: free surface calculations with ranse and level set method, dalida project* (No. INSEAN TR 2008-047). INSEAN.
- 172.** Brutti, S. (2008). *Metodi computazionali da principi primi nella scienza dei materiali*. Terzo Convegno Giovani Chimici. 18-19 Giugno 2008, Roma (IT).

- 173.** Burattini, P., Leonardi, S., Orlandi, P., & Antonia, R. A. (2008). Comparison between experiments and direct numerical simulations in a channel flow with roughness on one wall. *J. Fluid. Mech.*, **600**, 403-426.
- 174.** Caciatore, M., Rutigliano, M., Pieretti, A., Sanna, N., & Zazza, C. (2008). *Catalytic activity of silica surfaces in dissociated oxygen/nitrogen from ab initio calculations*. Sixth European Symposium on Aerothermodynamics for Space Vehicles, November 3-6, 2008, Versailles, France.
- 175.** Calzavarini, E., Kerscher, M., Lohse, D., & Toschi, F. (2008). Dimensionality and morphology of particle and bubble clusters in turbulent flow. *J. Fluid. Mech.*, **607**, 13-24.
- 176.** Capitani, G. C., Stixrude, L., & Mellini, M. (2008). *Ab initio quantum mechanical investigation of antigorite m = 17 structure and stability*. 2nd International Workshop: Layered Materials: Structure and Properties, Vercelli (IT).
- 177.** Capitani, G. C., Stixrude, L., & Mellini, M. (2008). *Total energies of different antigorite structure models: a dft study*. 1st SIMP-AIC joint meeting, Sestri Levante (GE), 7-12 Settembre 2008.
- 178.** Carelli, F., Sebastianelli, F., Baccarelli, I., & Gianturco, F. A. (2008). Following electron attachment to cs ((1)sigma): quantum scattering calculations of the lowest resonant state. *Int. J. Mass Spectrom.*, **277**(1-3), 155-161.
- 179.** Carey, R., Lucchese, R. R., & Gianturco, F. A. (2008). Positron scattering from c-20. *Phys. Rev. A*, **78**(1), 012706.
- 180.** Castrignanò, T., D'Antonio, M. R., Anselmo, A., Carrabino, D., D'Onorio De Meo, P., D'Ercchia, A. M., Licciulli, F., Mangiulli, M., Mignone, F., Pavese, G., Picardi, E., Riva, A., Rizzi, R., Bonizzoni, P. & Pesole, G. (2008). ASPicDB: A database resource for alternative splicing analysis. *Bioinformatics*, **24**(10), 1300-1304.
- 181.** Ceccarelli, M., Anedda, R., Casu, M., & Ruggerone, P. (2008). Co escape from myoglobin with metadynamics simulations. *Proteins: Structure Function And Bioinformatics*, **71**(3), 1231-1236.
- 182.** Ceccarelli, M., & Ruggerone, P. (2008). Physical insights into permeation of and resistance to antibiotics in bacteria. *Curr. Drug Targets*, **9**(9), 779-788.
- 183.** Chillemi, G., D'Annessa, I., Fiorani, P., Losasso, C., Benedetti, P., & Desideri, A. (2008). Thr729 in human topoisomerase I modulates anti-cancer drug resistance by altering protein domain communications as suggested by molecular dynamics simulations. *Nucleic Acids Res.*, **36**(17), 5645-5651.
- 184.** Ciamarra, M. P. & Coniglio, A. (2008). Random Very Loose Packings. *Phys. Rev. Lett.*, **101**(12), 12800.
- 185.** Coccia, E., Marinetti, F., Bodo, E., & Gianturco, F. A. (2008). Anionic microsolvation in helium droplets: oh-(he)(n) structures from classical and quantum calculations. *J. Chem. Phys.*, **128**(13), 134511.
- 186.** Coccia, E., Marinetti, F., Bodo, E., & Gianturco, F. A. (2008). Chemical solutions in a quantum solvent: anionic electrolytes in he-4 nanodroplets. *ChemPhysChem*, **9**(9), 1323-1330.
- 187.** Coccia, E., Bodo, E., Marinetti, F., Gianturco, F. A., Yurtsever, E., Yurtsever, M. & Yildirim, E. (2008). *Quantum structuring of ⁴He atoms around ionic dopants: energetics of Li⁺, Na⁺ and K⁺ from stochastic calculations*. ISAAC 2007 Conference Proceedings, Imperial College Press.
- 188.** Coccia, E., Bodo, E., & Gianturco, F. A. (2008). Nanoscopic phase changes in doped he-4 droplets. *Epl*, **82**(2), 23001.
- 189.** Colizzi, G., Filippetti, A., Cossu, F., & Fiorentini, V. (2008). Interplay of strain and magnetism in la1-xsrxmno3 from first principles. *Phys. Rev. B*, **78**(23), 235122.
- 190.** Conte, C., Gambardella, S., Bulli, C., Rinaldi, F., Di Marino, D., Falconi, M., et al. (2008). Screening of eda1 gene in x-linked anhidrotic ectodermal dysplasia using dhplc: identification of 14 novel mutations in italian patients. *Genet. Test.*, **12**(3), 437-442.
- 191.** Cox, K., Bond, P. J., Grottesi, A., Baaden, M. & Sansom, M. S. P. (2008). Outer membrane proteins: comparing X-ray and NMR structures by MD simulations in lipid bilayers. *Eur. Biophys. J.*, **37**(2), 131-141.
- 192.** Crescenzi, O., & Barone, V. (2008). *Applicazioni dell'hpc per la soft matter: fra scienze della vita e scienza dei materiali*. Italian e-Science 2008, Università degli Studi di Napoli Federico II, Napoli, 27-29 Maggio 2008.
- 193.** Crescenzi, O. (2008). *Computational spectroscopy of organic molecules - some case studies*. TheTIS Workshop, Ecole National Supérieure de Chimie de Paris, Paris, February 14-16, 2008.
- 194.** Crescenzi, O., & Barone, V. (2008). *In silico evaluation of nmr observables in biomolecules*. 7th European Conference on Computational Chemistry, Università degli Studi di Padova, San Servolo, Venezia (IT), 11-15 Settembre 2008.
- 195.** Cristiani, E., & Falcone, M. (2008). *Numerical solution of the isaacs equation for differential games with state constraints*. Proceedings of 17th IFAC World Congress, Seoul, Korea.
- 196.** Cruz Perez, B., Toro Medina, J., Thole, K., Sundaram, N., & Leonardi, S. (2008). *Direct numerical simulation and experimental results of a turbulent channel flow with pin fins array*. ERCOFATC Workshop, Direct and Large-Eddy Simulations 7 (DLSE7), September 8-10, 2008.
- 197.** D'Abromo, M., Aschi, M., Di Nola, A., & Amadei, A. (2008). The kinetics of carbon monoxide migration and binding in solvated myoglobin as revealed by molecular dynamics simulations, submitted.
- 198.** D'Abromo, M., Di Nola, A., Aschi, M., & Amadei, A. (2008). Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: comparison with recent experimental data. *J. Chem. Phys.*, **128**(2), 021103.

- 199.** D'Alessandro, M., Di Lella, A., Aschi, M., Di Nola, A., & Amadei, A. (2008). Theoretical characterization of structural and energetical properties of water clusters, by means of a simple polarizable water hamiltonian. *J. Mol. Liq.*, **142**(1-3), 111-117.
- 200.** D'Angelo, P., Migliorati, V., Mancini, G., & Chillemi, G. (2008). A coupled molecular dynamics and xanes data analysis investigation of aqueous cadmium(ii). *J. Phys. Chem. A*, **112**, 11833-11841.
- 201.** D'Angelo, P., De Panfilis, S., Filipponi, A., & Persson, I. (2008). High-energy x-ray absorption spectroscopy: a new tool for structural investigations of lanthanoids and third-row transition elements. *Chem-Eur. J.*, **14**, 3045-3055.
- 202.** D'Angelo, P., Migliorati, V., Mancini, G., Barone, V., & Chillemi, G. (2008). Integrated experimental and theoretical approach for the structural characterization of Hg(2+) aqueous solutions. *J. Chem. Phys.*, **128**(8), 084502.
- 203.** D'Angelo, P., Lapi, A., Migliorati, V., Arcovito, A., Benfatto, M., Roscioni, O. M., et al. (2008). X-ray absorption spectroscopy of hemes and hemeproteins in solution: multiple scattering analysis. *Inorg. Chem.*, **47**, 9905-9918.
- 204.** D'Angelo, P., Zitolo, A., Migliorati, V., & Pavel, N. V. (2008). X-ray multielectron photoexcitations at the i- k-edge. *Phys. Rev. B*, **78**, 144105.
- 205.** D'Ischia, M., Crescenzi, O., Pezzella, A., Arzillo, M., Panzella, L., Napolitano, A., & Barone, V. (2008). Structural effects on the electronic absorption properties of 5,6-dihydroxyindole oligomers: the potential of an integrated experimental and dft approach to model eumelanin optical properties. *Photochem. Photobiol.*, **84**(3), 600-607.
- 206.** Della Greca, M., Iesce, M. R., Previtera, L., Rubino, M., Barone, V., & Crescenzi, O. (2008). Phototransformation of the drug trazodone in aqueous solution. *J. Photoch. Photobio. A*, **199**(2-3), 353-357.
- 207.** Delugas, P., Fiorentini, V., & Filippetti, A. (2008). Dielectric constant boost in amorphous sesquioxides. *Appl. Phys. Lett.*, **92**(17), 172903.
- 208.** Di Valentin, M., Ceola, S., Agostini, G., Giacometti, G. M., Angerhofer, A., Crescenzi, O., et al. (2008). Pulse endor and density functional theory on the peridinin triplet state involved in the photo-protective mechanism in the peridinin-chlorophyll a-protein from amphidinium carterae. *BBA-Bioenergetics*, **1777**(3), 295-307.
- 209.** D'Onorio De Meo, P., Carrabino, D., D'Antonio, M. R., Sanna, N., Castrignanò, T., Maglietta, R., D'Addabbo, A., Liuni, S., Mignone, F., Pesole, G. & Ancona, N. (2008). HT-RLS: high-throughput web tool for analysis of DNA microarray data using RLS classifiers. *Cluster Computing and the Grid, IEEE International Symposium*, 747-752.
- 210.** Falcone, M., & Rorro, M. (2008). *On a variational approximation of the effective Hamiltonian*. Springer.
- 211.** Falconi, M., Oteri, F., Eliseo, T., Cicero, D. O., & Desideri, A. (2008). Md simulations of papillomavirus dna-e2 protein complexes hints at a protein structural code for dna deformation. *Biophys. J.*, **95**(3), 1108-1117.
- 212.** Filippetti, A., Lopez, G. M., Mantega, M., & Fiorentini, V. (2008). Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped yba₂cu₃o_{6+x}: a first principles description. *Phys. Rev. B*, **78**(23), 233103.
- 213.** Filippetti, A., & Fiorentini, V. (2008). Metal-insulator transitions and singlet polarons in one-dimensional ca_{2+xy2-x}cu₅o₁₀. *Phys. Rev. B*, **77**(23), 235124.
- 214.** Franz, J., Gianturco, F. A., Baluja, K. L., Tennyson, J., Carey, R., Montuoro, R., et al. (2008). Correlation-polarization effects in electron/positron scattering from acetylene: a comparison of computational models. *Nucl. Instrum. Meth. B*, **266**(3), 425-434.
- 215.** Galantini, L., Leggio, C., & Pavel, N. V. (2008). Human serum albumin unfolding: a small-angle x-ray scattering and light scattering study. *J. Phys. Chem. B*, **112**(48), 15460-15469.
- 216.** Gianturco, F. A. (2008). Quenching of internally 'hot' h-2 and n-2 gases by collisions with ultracold electrons: a computational 'experiment'. *Phys. Scr.*, **78**(5), 058102.
- 217.** Gianturco, F. A., Sebastianelli, F., Lucchese, R. R., Baccarelli, I., & Sanna, N. (2008). Ring-breaking electron attachment to uracil: following bond dissociations via evolving resonances. *J. Chem. Phys.*, **128**(17), 174302.
- 218.** Gonnella, G., Lamura, A., & Piscitelli, A. (2008). Dynamics of binary mixtures in inhomogeneous temperatures. *J. Phys. A: Math. Theor.*, **41**(10), 105001.
- 219.** Gontrani, L., Ramondo, F., Caracciolo, G., & Caminiti, R. (2008). A study of cyclohexane, piperidine and morpholine with x-ray diffraction and molecular simulations. *J. Mol. Liq.*, **139**, 23-28.
- 220.** Gonzalez-Sanchez, L., Tacconi, M., Bodo, E., & Gianturco, F. A. (2008). Ionic interactions and quenching dyn mics in cold traps: rotationally cooling collisions of oh^- ('s^+) with rb(^2 s). *Eur. Phys. J. D*, **49**, 85-92.
- 221.** Gonzalez-Sanchez, L., Bodo, E., Yurtsever, E., & Gianturco, F. A. (2008). Quenching efficiency of "hot" polar molecules by he buffer gas at ultralow energies: quantum results for mgh and lih rotations. *Eur. Phys. J. D*, **48**(1), 75-82.
- 222.** Gori, P., Contini, G., Prosperi, T., Ronci, F., Colonna, S., Zema, N., et al. (2008). Adsorption and self-assembly of d-alanine on cu(100). *Superlattice. Microst.*, in press.
- 223.** Gori, P., Contini, G., Prosperi, T., Catone, D., Turchini, S., Zema, N., & Palma, A. (2008). D-alanine adsorption on cu(100): photoelectron spectroscopy and first-principles calculations. *J. Phys. Chem. B*, **112**(13), 3963-3970.
- 224.** Gualtieri, P., Jacob, B., Casciola, C. M., & Piva, R. (2008). *The effect of shear on anisotropic fluctuations in a homogeneous shear flow* (Vol. 117) Springer Berlin-Heidelberg.

- 225.** Iafrati, A., & Broglia, R. (2008). *Hydrodynamics of planning hulls: a comparison between rans and 2d+t potential flows models.* 27th ONR Symposium on Naval Hydrodynamics, 5-10 October 2008, Seoul, Korea.
- 226.** Iemma, U. (2008). *Singing integrals or wind instrument modeling using boundary integral equations.* Acoustics'08, 29/06-04/07, Paris, France.
- 227.** Inghilesi, R., Stocca, V., Roman, F. & Armenio, V. (2008). Dispersion of a vertical jet of buoyant particles in a stably stratified wind-driven Ekman layer. *Int. J. Heat Fluid Fl.*, **29**(3), 733-742.
- 228.** Ippolito, M., Meloni, S., & Colombo, L. (2008). Interface structure and defects of silicon nanocrystals embedded into a-sio2. *Appl. Phys. Lett.*, **93**(15), 153109.
- 229.** Kalitzova, M., Lebedev, O. I., Zollo, G., Gesheva, K., Vlakhov, E., Marinov, Y., & Ivanova, T. (2008). Dynamics of nanoclustering in te+ implanted si after application of high frequency electromagnetic field and thermal annealing. *Appl. Phys. A-Mater.*, **91**(3), 515-519.
- 230.** Labro, A., Grottesi, A., Sansom, M. S. P., Raes, A. & Snyders, D. (2008). A Kv channel with an altered activation gate sequence displays both "fast" and "slow" activation kinetics. *Am. J. Physiol. Cell Physiol.*, **294**(6), C1476-C1484.
- 231.** Labro, A., Raes, A., Grottesi, A., Hoorick, D. V., Sansom, M. S. P. & Snyders, D. (2008). Kv channel gating requires a compatible S4-S5 linker and bottom part of S6, constrained by non-interacting residues. *J. Gen. Physiol.*, **132**(6), 667-680.
- 232.** Leggio, C., Galantini, L., & Pavel, N. V. (2008). About the albumin structure in solution: cigar expanded form versus heart normal shape. *Phys. Chem. Chem. Phys.*, **10**, 6741-6750.
- 233.** Leonardi, S., & Castro, I. (2008). Direct numerical simulation of the turbulent flow over an urban canopy made of cubical obstacles. *APS Meeting Abstracts*.
- 234.** Leonardi, S., & Castro, I. (2008). *Turbulent flow over urban canopies.* 5th AIAA Theoretical Fluid Mechanics Conference, June 23-26, 2008.
- 235.** Leonelli, F., Capuzzi, M., Bodo, E., Passacantilli, P. & Piancatelli, G. (2008). Synthesis of new 2-Phosphono-alpha-D-Glycoside derivatives by stereoselective Oxa-Michael addition to D-Galacto derived enone. *Carbohydr. Res.*, **343**, 1133-1135.
- 236.** Liberati, A., & Okuno, Y. (2008). Improvement of plasma-flow behavior and performance of a disk mhd generator under high magnetic flux densities. *IEE Trans. Power Energ.*, **128**(2), 493-498.
- 237.** Liberati, A., & Okuno, Y. (2008). *Numerical simulation of high mach number - low static pressure plasma in a highly efficient disk mhd generator.* Proceedings of the 38th AIAA Plasmadynamics and Lasers Conference. June 23-26, 2008.
- 238.** Liberati, A., Murakami, T., Okuno, Y., & Yamasaki, H. (2008). *Numerical simulation of mhd flow and heat transfer in the disk mhd generator of closed loop experimental facility at tokyo tech.* Proceedings of the 7th PAMIR International Conference in Fundamental and Applied MHD. September 8-12, 2008.
- 239.** Liberati, A., Ohno, J., Murakami, T., & Okuno, Y. (2008). *Numerical study of plasma-fluid behavior and generation characteristics of the closed loop mhd power generator.* Proceedings of the 3rd New Energy Symposium. March 14-15, 2008.
- 240.** Lopez-Duran, D., Bodo, E., & Gianturco, F. A. (2008). Aspin: an all spin scattering code for atom-molecule rovibrationally inelastic cross sections. *Comput. Phys. Commun.*, **179**(11), 821-838.
- 241.** Losasso, C., Cretaio, E., Fiorani, P., D'Annessa, I., Chillemi, G. & Benedetti, P. (2008). A single mutation in the 729 residue modulates human DNA topoisomerase IB DNA binding and drug resistance. *Nucleic Acids Res.*, **36**(17), 5635-5644.
- 242.** Lotito, L., Russo, A., Chillemi, G., Bueno, S., Cavalieri, D., & Capranico, G. (2008). Global transcription regulation by DNA topoisomerase I in exponentially growing *Saccharomyces cerevisiae* cells: activation of telomere-proximal genes by TOP1 deletion. *J. Mol. Biol.*, **377**(2), 311-322.
- 243.** Mach, T., Neves, P., Spiga, E., Weingart, H., Winterhalter, M., Ruggerone, P., et al. (2008). Facilitated permeation of antibiotics across membrane channels - interaction of the quinolone moxifloxacin with the ompf channel. *J. Am. Chem. Soc.*, **130**(40), 13301-13309.
- 244.** Mancini, G., Sanna, N., Barone, V., Migliorati, V., D'Angelo, P., & Chillemi, G. (2008). Structural and dynamical properties of the hg(2+) aqua ion: a molecular dynamics study. *J. Phys. Chem. B.*, **112**, 4694-4702.
- 245.** Manini, P., Capelli, L., Reale, S., Arzillo, M., Crescenzi, O., Napolitano, A., et al. (2008). Chemistry of nitrated lipids: remarkable instability of 9-nitrolinoleic acid in neutral aqueous medium and a novel nitronitrate ester product by concurrent autoxidation/nitric oxide-release pathways. *J. Org. Chem.*, **73**(19), 7517-7525.
- 246.** Marinetti, F., Bodo, E., Gianturco, F. A., & Yurtsever, E. (2008). Energetics and structures of charged helium clusters: comparing stabilities of dimer and trimer cationic cores. *ChemPhysChem*, **9**(17), 2618-2624.
- 247.** Martinelli, S., Torrieri, P., Stella, L., Bocchinfuso, G., Flex, E., Grottesi, A., et al. (2008). Diverse driving forces underlie the invariant occurrence of t42a, e139d, i282v and t468m shp2 amino acid substitution causing noonan and leopard syndromes. *Hum. Mol. Genet.*, **17**, 2018-2029.
- 248.** Mattoni, A., & Colombo, L. (2008). Crystallization kinetics of mixed amorphous-crystalline nanosystems. *Phys. Rev. B.*, **78**(7), 075408.

- 249.** Monteferrante, M., Bonella, S., Meloni, S., Vanden-Eijnden, E., & Ciccotti, G. (2008). Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. *Sci. Model. Simul.*, **15**, 187-206.
- 250.** Muscari, R., Broglia, R., & Di Mascio, A. (2008). *Analysis of the flow around a manoeuvring vlcc*. OMAE 2008, 27th International Conference on Offshore Mechanics and Arctic Engineering, June 15-20, 2008, Estoril (Portugal).
- 251.** Muscari, R., Di Mascio, A., & Broglia, R. (2008). *Sviluppo di un codice di calcolo per la simulazione di flussi non stazionari ad elevato numero di reynolds intorno a carene navali con appendici mobili e propulsore. LottoE: simulazione degli organi di governo di una carena navale di tipo militare, mobiprop project* (No. INSEAN TR 2008-020). INSEAN.
- 252.** Muscari, R., Di Mascio, A., & Broglia, R. (2008). *Sviluppo di un codice di calcolo per la simulazione di flussi non stazionari ad elevato numero di reynolds intorno a carene navali con appendici mobili e propulsore. Lotto F: simulazione del flusso intorno ad un propulsore dietro carena, mobiprop project*, (No. INSEAN TR 2008-033). INSEAN.
- 253.** Muscari, R., Broglia, R., & Di Mascio, A. (2008). *Trajectory prediction of a self propelled hull by unsteady rans computations*. 27th ONR Symposium on Naval Hydrodynamics, October 5-10, 2008, Seoul, Korea.
- 254.** Napoli, I., Mercaldo, V., Boyl, P. P., Eleuteri, B., Zalfa, F., De Rubeis, S., et al. (2008). The fragile x syndrome protein represses activity-dependent translation through cyfip1, a new 4e-bp. *Cell*, **134**(6), 1042-1054.
- 255.** Narzi, D., Daidone, I., Amadei, A., & Di Nola, A. (2008). Protein folding pathways revealed by essential dynamics sampling. *J. Chem. Theory Comput.*, **4**(11), 1940-1948.
- 256.** Noe, F., Daidone, I., Smith, J. C., Di Nola, A., & Amadei, A. (2008). Solvent electrostriction-driven peptide folding revealed by quasi-gaussian entropy theory and molecular dynamics simulation. *J. Phys. Chem. B*, **112**(35), 11155-11163.
- 257.** Ohno, J., Liberati, A., Murakami, T., & Okuno, Y. (2008). Numerical study of plasma-fluid behavior and generation characteristics of the closed loop mhd electrical power generator. *IEEJ Trans. Power Energ.*, **128**(11), 1401-1406.
- 258.** Orioni, B., Bocchinfuso, G., Kim, J. Y., Bobone, S., Venanzi, M., Palleschi, A., et al. (2008). *Localization of the antimicrobial peptide pmap-23 in lipid bilayer implications for the mechanism of action*. 1st "the First Italy-Korea Symposium on Antimicrobial Peptides (8th RCPM International Symposium)". Seosuk Hall, Chosun University, Gwangju, Korea July 24-25, 2008.
- 259.** Orioni, B., Bocchinfuso, G., Kim, J. Y., Grande, G., Bobone, S., Venanzi, M., et al. (2008). *Localization of the antimicrobial peptide pmap-23 in phospholipid membranes. a combined spectroscopic and molecular dynamics study*. XXXVII Congresso Nazionale di Chimica Fisica, 24-29 Febbraio 2008, Camogli, Genova (IT).
- 260.** Orlandi, P., & Leonardi, S. (2008). Direct numerical simulation of three-dimensional turbulent rough channels: parameterization and flow physics. *J. Fluid Mech.*, **606**, 399-415.
- 261.** Orlandi, P. (2008). Vorticity dynamics in turbulence growth. *APS Meeting Abstracts*.
- 262.** Orlandini, S., Baccarelli, I., & Gianturco, F. A. (2008). Searching for many-body effects and efimov states in very weakly bound triatomics: heneh- and heneh. *Mol. Phys.*, **106**(2-4), 573-586.
- 263.** Paci, P., Castiglione, F., Bernaschi, M., & Baldazzi, V. (2008). *A discrete/continuous model of anti-hiv response and therapy*. Tenth International Conference on Computer Modeling and Simulation, 2008. UKSIM 2008.
- 264.** Pariset, L., Bongiorni, S., Chillemi, G., Prosperini, G., Bueno, S., Signorelli, F., Moioli, B. & Valentini, A. (2008). Transcriptomic analysis of two sheep breeds during lactation, using a new custom microarray platform. *Ital. J. Anim. Sci.*, **6**(Supp. 1), 182.
- 265.** Pariset, L., Bueno, S., Prosperini, G., Chillemi, G., Gentile, A. & Valentini, A. (2008). *Metabolic pathways affected by spastic paresis in cattle*. XLIII International Animal Production Symposium on nutripharm & biosecurity.
- 266.** Pariset, L., Chillemi, G., Bueno, S., Prosperini, G., Bongiorni, S. & Valentini, A. (2008). *A tool for quality and safety projects: custom microarray from public databases*. XLIII International Animal Production Symposium on nutripharm & biosecurity.
- 267.** Pariset, L., Chillemi, G., Bueno, S., Prosperini, G., Bongiorni, S. & Valentini, A. (2008). *From public sequences to custom microarrays: an easy and affordable tool*. XXXI conference of the international society for animal genetics.
- 268.** Pellegrino, M., Apollonio, F., Liberti, M., Amadei, A., Di Nola, A. & D'Inzeo, G. (2008). *Molecular simulations of biochemical processes in presence of a MW signal*. IEEE Antennas and Propagation Society International Symposium, **1-9**, 2990-2993.
- 269.** Persson, I., D'Angelo, P., De Panfilis, S., Sandstrom, M., & Eriksson, L. (2008). Hydration of lanthanoid(III) ions in aqueous solution and crystalline hydrates studied by exafs spectroscopy and crystallography: the myth of the gadolinium break. *Chem-Eur. J.*, **14**, 3056-3066.
- 270.** Picano, F., Casciola, C. M., & Hanjalic, K. (2008). *Scrutinizing the leray-alpha regularization for les in turbulent axysymmetric free jets*. ERCOFTAC Workshop, Direct and Large-Eddy Simulations 7 (DLSE7), September 8-10, 2008.
- 271.** Piccinini, E., Ceccarelli, M., Affinito, F., Brunetti, R., & Jacoboni, C. (2008). Biased molecular dynamics simulations for free-energy mapping: a comparison on the kcsa channel as a test case. *J. Chem. Theory Comput.*, **5**, 173-183.
- 272.** Pirozzoli, S., Bernardini, M., & Grasso, F. (2008). Characterization of coherent vortical structures in a supersonic turbulent boundary layer. *J. Fluid. Mech.*, **613**, 205-231.
- 273.** Roman, F., Armenio, V., Inghilesi, R., & Corsini, S. (2008). *Large eddy simulation of turbulent mixing in an estuary region*. ERCOFTAC Workshop, Direct and Large-Eddy Simulations 7 (DLSE7), September 8-10, 2008.

- 274.** Rorro, M., Numerical Methods for the Effective Hamiltonian on Serial and Parallel Machines (2008). Università degli Studi di Roma "La Sapienza", Dottorato di Ricerca in "Metodi e Modelli Matematici per la Tecnologia e la Società".
- 275.** Sameen, A., Verzicco, R., & Sreenivasan, K. R. (2008). Non-boussinesq convection at moderate rayleigh numbers in low temperature gaseous helium. *Phys. Scripta*, **T132**, 014053.
- 276.** Sánchez Garrido, J. C., García Lafuente, J., Criado Aldeanueva, F., Baquerizo, A., & Sannino, G. (2008). Time-spatial variability observed in velocity of propagation of the internal bore in the strait of gibraltar. *J. Geophys. Res.*, **113**, C07034.
- 277.** Sannino, G., Herrmann, M., Carillo, A., Rupolo, V., Ruggiero, V., Artale, V., & Heimbach, P. (2008). An eddy-permitting model of the mediterranean sea with a two-way grid refinement at gibraltar. *Ocean Modeling*, in press.
- 278.** Sardina, G., Gualtieri, P., & Casciola, C. M. (2008). Unconfined isotropic turbulence in time-decay. *APS Meeting Abstracts*.
- 279.** Silano, G. (2008). Numerical simulations of thermal convection at high prandtl numbers. *APS Meeting Abstracts*.
- 280.** Silano, G., Sreenivasan, K. R., & Verzicco, R. (2008). *Numerical simulations of thermal convection at high prandtl numbers*. Ercoftac Workshop, Direct and Large-Eddy Simulations 7 (DLSE7), September 8-10, 2008.
- 281.** Spiegel, K., Magistrato, A., Maurer, P., Ruggerone, P., Rothlisberger, U., Carloni, P., Reedijk, J. & Klein, M. L. (2008). Parameterization of azole-bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. *J. Comput. Chem.*, **29**(1), 38-49.
- 282.** Stansfeld, P. J., Grottesi, A., Sands, Z. A., Sansom, M. S. P., Gedeck, P., Gosling, M., Cox, B., Stanfield, P. R., Mitcheson, J. S. & Sutcliffe, M. J. (2008). Insight into the mechanism of inactivation and pH sensitivity in potassium channels from molecular dynamics simulations. *Biochemistry*, **47**(28), 7414-7422.
- 283.** Stella, L., Bocchinfuso, G., Orioni, B., Bobone, S., Mazzuca, C., Venanzi, M., & Palleschi, A. (2008). *Characterization of peptide-membrane interactions by fluorescence spectroscopy and molecular dynamics simulations*. Convegno Società Italiana di Biofisica Pura e Applicata, Roma, Settembre 2008.
- 284.** Stella, L., Bocchinfuso, G., Grande, G., Orioni, B., Venanzi, M., Kim, J. Y., et al. (2008). Determining the location of antimicrobial peptides inside lipid bilayers by combined fluorescence spectroscopy and molecular dynamics simulations. *European Peptide Society*, in press.
- 285.** Sterpone, F., Spanu, L., Ferraro, L., Sorella, S., & Guidoni, L. (2008). Dissecting the hydrogen bond: a quantum monte carlo approach. *J. Chem. Theory Comput.*, **4**(9), 1428-1434.
- 286.** Tacconi, M., & Gianturco, F. A. (2008). Molecular ions in ultracold atomic gases: computed electronic interactions for mgh+(x-1 sigma(+)) with rb. *Eur. Phys. J. D*, **46**(3), 443-451.
- 287.** Tai, K., Haider, S., Grottesi, A., & Sansom, M. S. P. (2008). Ion channels gates: comparative analysis of energy barriers. *Eur. Biophys. J.*, **38**, 347-354.
- 288.** Torre, M., Manno, V., Allepuz, A., Behar, S., Bellocchio, R., Fusco, D., et al. (2008). *The euphoric project: outcome indicators collection in europe. Results of the second phase (pilot)*. European Journal of Public Health, Lisbon.
- 289.** Valentini, A., Castrignanò, T., Bueno, S., Carrabino, D., Pariset, L., Paoletti, D. & Chillemi, G. (2008). *Dynamic annotation of dna sequences in agricultural species*. XXXI Conference of the International Society for Animal Genetics.
- 290.** Vargiu, A. V., Robertazzi, A., Magistrato, A., Ruggerone, P. & Carloni, P. (2008). The hydrolysis mechanism of the anticancer rutenium drugs NAMI-A and ICR investigated by DFT-PCM calculations. *J. Phys. Chem. B*, **112**(14), 4401-9.
- 291.** Vargiu, A. V., Ruggerone, P., Magistrato, A., & Carloni, P. (2008). Dissociation of minor groove binders from dna: insights from metadynamics simulations. *Nucleic Acids Res.*, **36**(18), 5910-5921.
- 292.** Vargiu, A. V., Ruggerone, P., Magistrato, A., & Carloni, P. (2008). Sliding of alkylating anticancer drugs along the minor groove of dna: new insights on sequence selectivity. *Biophys. J.*, **94**(2), 550-561.
- 293.** Verzicco, R., & Sreenivasan, K. R. (2008). A comparison of turbulent thermal convection between conditions of constant temperature and constant heat flux. *J. Fluid Mech.*, **595**, 203-219.
- 294.** Verzicco, R. (2008). *Numerical experiments on turbulent thermal convection*. Ercoftac Workshop, Direct and Large-Eddy Simulations 7 (DLSE7), September 8-10, 2008.
- 295.** Volk, R., Calzavarini, E., Verhille, G., Lohse, D., Mordant, N., Pinton, J.-F., & Toschi, F. (2008). Acceleration of heavy and light particles in turbulence: comparison between experiments and direct numerical simulations. *Physica D: Nonlinear Phenomena*, **237**(14-17), 2084-2089.
- 296.** Volodin, E. M., Diansky, N. A., Lanucara, P., Purini, R. & Transerici, C. (2008). Climate variations in the Northern Hemisphere based on the use of an atmosphere-ocean IPCC model. *Il Nuovo Cimento C*, **31**(2).
- 297.** Xiong, K., Delugas, P., Hooker, J. C., Fiorentini, V., Robertson, J., Liu, D. M., & Pourtois, G. (2008). Te-induced modulation of the mo/hfo₂ interface effective work function. *Appl. Phys. Lett.*, **92**(11), 113504.
- 298.** Zaghi, S., Favini, B., Di Giacinto, M., & Serraglia, F. (2008). *3d simulations of pre-ignition transient of p80 srm*. 44th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit.
- 299.** Zaghi, S., Favini, B., & Di Giacinto, M. (2008). *Ignition transient of vega's solid rocket motors*. 2nd International Symposium on Propulsion for Space Transportation, May 5-9, 2008.

- 300.** Zanetti-Polzi, M., Anselmi, M., D'Alessandro, A., Amadei, A., & Di Nola, A. (2008). Structural, thermodynamic and kinetic properties of gramicidin analogue gs6 studied by molecular dynamics simulations and statistical mechanics, submitted.
- 301.** Zazza, C., Amadei, A., Sanna, N., & Aschi, M. (2008). Can a synthetic thread act as an electrochemically switchable molecular device? *Chem. Commun.*, **29**, 3399-3401.
- 302.** Zazza, C., Rutigliano, M., Cacciatore, M., Mancini, G., Pieretti, A., & Sanna, N. (2008). *Electronic structure calculations and collision dynamics for the interaction of o atoms with two sio₂ polymorphs*. ECOSS 25, European Conference on Surface Science, Liverpool, July 31-August 1, 2008.
- 303.** Zazza, C., Meloni, S. & Palma, A. (2008). Structural and electronic properties of metal doped organic semiconductors. *Mod. Phys. Lett. B*, **22**(17), 1609-1631.
- 304.** Zazza, C., Amadei, A., Palma, A., Sanna, N., Tatoli, S., & Aschi, M. (2008). Theoretical modeling of enzyme reactions: the thermodynamics of formation of compound 0 in horseradish peroxydase. *J. Phys. Chem. B*, **112**, 3184-3192.
- 305.** Zollo, G., & Gala, F. (2008). Properties of charged intrinsic di-interstitials in gaas. *Phys. Rev. B*, **77**, 094125.

2007

- 306.** Acebron, J. A., & Spigler, R. (2007). *A fully scalable parallel algorithm for solving elliptic partial differential equations* (Vol. 4641) Springer Berlin-Heidelberg.
- 307.** Acebron, J. A., & Spigler, R. (2007). *A new probabilistic approach to the domain decomposition method* (Vol. 55). New York: Springer Berlin-Heidelberg.
- 308.** Acebron, J. A., & Spigler, R. (2007). Supercomputing applications to the numerical modeling of industrial and applied mathematics problems. *J. Supercomput.*, **40**(1), 67-80.
- 309.** Amati, G. (2007). *A three years experience with nec sx-6+ at caspur*. Nec User Group -XIX General Meeting Workshop, May 2007.
- 310.** Amati, F., Biancolella, M., Farcomeni, A., Giallonardi, S., Bueno, S., Minella, D., et al. (2007). Dynamic changes in gene expression profiles of 22q11 and related orthologous genes during mouse development. *Gene*, **391**(1-2), 91-102.
- 311.** Amati, G., Koal, K., Massaioli, F., Sreenivasan, K. R., & Verzicco, R. (2007). *Numerical experiments of turbulent thermal convection at high rayleigh numbers* (Vol. 109) Springer Berlin-Heidelberg.
- 312.** Araya, G., Leonardi, S., Castillo, L., & Orlandi, P. (2007). Direct numerical simulations of a passive scalar in a turbulent channel with local forcing at walls. *Int. J. Transport Phenomena*, **9**(4), 297-310.
- 313.** Arcovito, A., Benfatto, M., Della Longa, S., & D'Angelo, P. (2007). Hemeproteins: recent advances in quantitative xanes analysis. *AIP Conf. Proc.*, **882**, 306-310.
- 314.** Aurisicchio, C., Baciocchi, E., Gerini, M. F., & Lanzalunga, O. (2007). Thermal and Photochemical Racemization of Chiral Aromatic Sulfoxides via the Intermediacy of Sulfoxide Radical Cations. *Org. Lett.*, **9**(10), 1939-1942.
- 315.** Baccarelli, I., Gianturco, F. A., Grandi, A., Lucchese, R. R., & Sanna, N. (2007). Electron-driven molecular processes induced in biological systems by electromagnetic and other ionizing sources. *Adv. Quantum Chem.*, **52**, 189-230.
- 316.** Baccarelli, I., Gianturco, F. A., Grandi, A., Sanna, N., Lucchese, R. R., Bald, I., et al. (2007). Selective Bond Breaking in beta-D-Ribose by Gas-Phase Electron Attachment around 8 eV. *J. Am. Chem. Soc.*, **129**(19), 6269-6277.
- 317.** Bemporad, D., Sands, Z. A., Wee, C.-L., Grottesi, A., & Sansom, M. S. P. (2007). Vstx1, a modifier of kv channel gating, localizes to the interfacial region of lipid bilayers. *Biochemistry*, **45**, 11844-11855.
- 318.** Bersani, A. M., Lanucara, P., Rorro, M., & Ruggiero, V. (2007). *Systems biology and advanced computing*. MASCOT07 Proceedings, MASCOT07-IMACS/ISGG Workshop, IAC-CNR, Rome (IT).
- 319.** Biancolella, M., Valentini, A., Minella, D., Vecchione, L., D'Apice, M. R., Chillemi, G., et al. (2007). Effects of dutasteride on the expression of genes related to androgen metabolism and related pathway in human prostate cancer cell lines. *Invest New Drugs*, **25**(5), 491-497.
- 320.** Broglia, R., Di Mascio, A., & Amati, G. (2007). *A parallel unsteady rans code for the numerical simulations of free surface flows*. 2th International Conference on Marine Research and Trasportation, 28-30 Giugno 2007, Ischia, Naples (IT).
- 321.** Broglia, R., Di Mascio, A., & Muscari, R. (2007). Numerical study of confined water effects on self-propelled submarine in steady manoeuvres. *Int. J. Offshore Polar Eng.*, **17**(2), 89-96.
- 322.** Broglia, R., Muscari, R., Di Mascio, A., Bouscasse, B., Binotti, E., & Grizzi, S. (2007). *Submarine motions in confined waters, technical report n.8, euclid 10.17 project* (No. INSEAN TR 2007-011). INSEAN.
- 323.** Broglia, R., Di Mascio, A., & Amati, G. (2007). *Xnavis: a parallel cfd code for numerical simulation of unsteady free surface flows for naval hydrodynamics*. CAPI 2007 - Convegno Calcolo ad Alte Prestazioni in Italia, 15 - 16 Ottobre 2007, Politecnico di Milano, Milano (IT).
- 324.** Cabella, P., Natoli, P., & Silk, J. (2007). Constraints on cpt violation from wilkinson microwave anisotropy probe three year polarization data: a wavelet analysis. *Phys. Rev. D*, **76**(12), 123014.
- 325.** Caccia, B., Mattia, M., Amati, G., Andenna, C., Benassi, M., D'Angelo, A., et al. (2007). Monte carlo in radiotherapy: experience in a distributed computational environment. *J. Phys.: Conf. Ser.*, **74**, 021001.

- 326.** Capitani, G. C., Stixrude, L., & Mellini, M. (2007). *First principles energetics and structural relaxation of antigorite m = 17*. 1st Meeting of the Italian and Spanish Crystallographic Associations (MISCA), September 24-28, 2007, Villaggio Guglielmo, Copanello di Stalettì, Catanzaro (IT).
- 327.** Carbone, M., Palma, A., & Caminiti, R. (2007). C(1s) core-level photoemission spectra of stilbene on si (100) 2x1 surface from first-principles calculations. *Phys. Rev. B*, **75**(24), 24532.
- 328.** Carbone, M., Meloni, S., & Caminiti, R. (2007). Dissociative versus molecular adsorption of phenol on si(100)2x1: a first-principles calculation. *Phys. Rev. B*, **76**(8), 08532.
- 329.** Carlini, E., Falcone, M., & Ferretti, R. (2007). A semi-lagrangian scheme for the curve shortening flow in codimension-2. *J. Comput. Phys.*, **225**(2), 1388-1408.
- 330.** Carrabino, D., D'Onorio De Meo, P., Sanna, N., Castrignanò, T., Orsini, M., Floris, M., & Tramontano, A. (2007). The mepsmap server. mapping epitopes on protein surface: mining annotated proteins. *IEEE T. NanoBioscience*, **6**(2), 155-161.
- 331.** Casciola, C. M., & De Angelis, E. (2007). Energy transfer in turbulent polymer solutions. *J. Fluid. Mech.*, **581**, 419-436.
- 332.** Casciola, C. M., Gualtieri, P., Jacob, B., & Piva, R. (2007). The residual anisotropy at small scales in high shear turbulence. *Phys. Fluids*, **19**(10), 101704.
- 333.** Castrignanò, T., D'Onorio De Meo, P., Carrabino, D., Orsini, M., Floris, M., & Tramontano, A. (2007). The MEPS server for identifying protein conformational epitopes. *BMC Bioinformatics*, **8 Suppl 1**, S6.
- 334.** Chillemi, G., Mancini, G., Sanna, N., Barone, V., Della Longa, S., Benfatto, M., et al. (2007). Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion. *J. Am. Chem. Soc.*, **129**(17), 5430-5436.
- 335.** Chillemi, G., Fiorani, P., Bruselles, A., Castelli, S., Campagna, A., Sarra, O., et al. (2007). Role of flexibility and long range communication on the function of human topoisomerase i. *Ital. J. Biochem.*, **56**(6), 110-114.
- 336.** Chillemi, G., Bruselles, A., Fiorani, P., Bueno, S., & Desideri, A. (2007). The open state of human topoisomerase I as probed by molecular dynamics simulation. *Nucleic Acids Res.*, **35**(9), 3032-3038.
- 337.** Coccia, E., Bodo, E., Marinetti, F., Gianturco, F. A., Yildrim, E., Yurtsever, M., & Yurtsever, E. (2007). Bosonic helium droplets with cationic impurities: onset of electrostriction and snowball effects from quantum calculations. *J. Chem. Phys.*, **126**(12), 124319.
- 338.** Colizzi, G., Filippetti, A., & Fiorentini, V. (2007). Magnetism of la0.625sr0.375mno3 under high pressure from first principles. *Phys. Rev. B*, **76**(6), 064428.
- 339.** Conti, M., Di Pietro, R., & Mancini, L. V. (2007). Ecce: enhanced cooperative channel establishment for secure pair-wise communication in wireless sensor networks. *Ad Hoc Netw.*, **5**(1), 49-62.
- 340.** Conti, M., Di Pietro, R., & Mancini, L. V. (2007). *Ripp-fs: an rfid identification, privacy preserving protocol with forward secrecy*. In Proceedings of the 3rd IEEE International Workshop on Pervasive Computing and Communication Security.
- 341.** Cox, K., Bond, P. J., Grottesi, A., Baaden, M., & Sansom, M. S. P. (2007). Outer membrane proteins: comparing x-ray and nmr structures by md simulations. *Eur. Biophys. J.*, **37**, 131-141.
- 342.** D'Ambra, P., Di Serafino, D., & Filippone, S. (2007). On the development of psblas-based parallel two-level schwarz preconditioners. *Appl. Numer. Math.*, **57**(11-12), 1181-1196.
- 343.** D'Onorio De Meo, P., Carrabino, D., Sanna, N., Castrignanò, T., Grillo, G., Licciulli, F., et al. (2007). A high performance grid web service framework for the identification of conserved sequence tags. *Future Gener. Comp. Sy.*, **23**(3), 371-381.
- 344.** Dal Peraro, M., Ruggerone, P., Raugei, S., Gervasio, F. L., & Carloni, P. (2007). Investigating biological systems using first principles car-parrinello molecular dynamics simulations. *Curr. Opin. Struct.*, **17**(2), 149-156.
- 345.** De Lucia, M., Mainieri, F., Verotta, L., Maffei, M., Panzella, L., Crescenzi, O., et al. (2007). Nitration versus nitrosation chemistry of menthofuran: remarkable fragmentation and dimerization pathways and expeditious entry into dehydromenthofurolactone. *J. Org. Chem.*, **72**(26), 10123-10129.
- 346.** De Troia, G., Ade, P. A. R., Bock, J. J., Bond, J. R., Borrill, J., Boscaleri, A., et al. (2007). Searching for non-gaussian signals in the boomerang 2003 cmb map: preliminary results. *New Astron. Rev.*, **51**(3-4), 250-255.
- 347.** De Troia, G., Ade, P. A. R., Bock, J. J., Bond, J. R., Borrill, J., Boscaleri, A., et al. (2007). Searching for non-gaussian signals in the boomerang 2003 cmb maps. *Astrophys. J.*, **670**(2), L73-L76.
- 348.** Delugas, P., Fiorentini, V., Filippetti, A., & Pourtois, G. (2007). Cation charge anomalies and high-k dielectric behavior in dysco3: ab initio density-functional and self-interaction-corrected calculations. *Phys. Rev. B*, **75**(11), 115126.
- 349.** Delugas, P., Fiorentini, V., & Filippetti, A. (2007). Conservation of dielectric constant upon amorphization in perovskite oxides. *Phys. Rev. B*, **76**(10), 104112.
- 350.** Delugas, P., Fiorentini, V., & Filippetti, A. (2007). Dielectric properties of rare-earth oxides: general trends from theory. *Top. Appl. Phys.*, **106**, 225-246.
- 351.** Di Mascio, A., Broglia, R., & Muscari, R. (2007). *Numerical simulations of viscous flow around a fully appended hull with enforced motion*. 9th International Conference on Numerical Ship Hydrodynamics, August 2007, Ann Arbor, Michigan (USA).

- 352.** Di Mascio, A., Broglia, R., & Muscari, R. (2007). On the application of the single-phase level set method to naval hydrodynamic flows. *Comput. Fluids*, **36**(5), 868-886.
- 353.** Eriksson, L., D'Angelo, P., Persson, I., & Lundberg, D. (2007). A structural study of the n,n'-dimethylpropyleneurea solvated zinc(ii) and cadmium(ii) ions in solution and crystalline state. *J. Mol. Liq.*, **131**, 105-112.
- 354.** Fachin, S. (2007). Long-run trends in internal migrations in italy: a study in panel cointegration with dependent units. *J. Appl. Econom.*, **22**(2), 401-428.
- 355.** Fachin, S., & Gavosto, A. (2007). The decline in italian productivity: a study in estimation of long-run trends in total factor productivity with panel cointegration methods. *Luiss Lab of European Economics - LLEE Working Document*(50).
- 356.** Falconi, M., Santolamazza, A., Eliseo, T., De Prat-Gay, G., Cicero, D. O., & Desideri, A. (2007). Molecular dynamics of the dna-binding domain of the papillomavirus e2 transcriptional regulator uncover differential properties for dna target accommodation. *FEBS J.*, **274**(9), 2385-2395.
- 357.** Falconi, M., Biocca, S., Novelli, G., & Desideri, A. (2007). Molecular dynamics simulation of human lox-1 provides an explanation for the lack of oxldl binding to the trp150ala mutant. *BMC Structural Biology*, **7**, 73.
- 358.** Filippetti, A., & Fiorentini, V. (2007). Magnetic ordering under strain and spin-peierls dimerization in gecuo3. *Phys. Rev. Lett.*, **98**(19), 196403.
- 359.** Filippetti, A., & Fiorentini, V. (2007). Self-interaction-free density-functional band theory for magnetic cuprates. *J. Magn. Magn. Mater.*, **310**(2 Part 2), 1648-1650.
- 360.** Fiorentini, V., Delugas, P., & Filippetti, A. (2007). *A theoretical view on the dielectric properties of crystalline and amorphous high- materials and films* (Vol. 27) Springer Berlin-Heidelberg.
- 361.** García Lafuente, J., Sánchez Roman, A., Díaz del Río, G., Sannino, G., & Sánchez Garrido, J. C. (2007). Recent observations of seasonal variability of the mediterranean outflow in the strait of gibraltar. *J. Geophys. Res.*, **112**, C10005.
- 362.** Geron, M., Paciorri, R., & Nasuti, F. (2007). Flowfield analysis of a linear clustered plug nozzle with round-to-square modules. *Aerosp. Sci. Technol.*, **11**(2-3), 110-118.
- 363.** Geron, M., Paciorri, R., & Nasuti, F. (2007). Performance analysis of an infinite array linear clustered plug nozzle. *J. Propul. Power*, **23**(1), 246-249.
- 364.** Gianturco, F. A., & Stoecklin, T. (2007). Electron scattering from gaseous ocs ((1)sigma): comparing computed angular distributions and elastic cross-sections with experiments. *Chem. Phys.*, **332**(2-3), 145-151.
- 365.** Gianturco, F. A., & Stoecklin, T. (2007). Low-energy electron scattering from gaseous cs2: angular distributions and effect of exchange forces. *Eur. Phys. J. D*, **42**(1), 85-91.
- 366.** Gianturco, F. A., & Willner, K. (2007). Ramsauer-townsend effect for electron scattering from gaseous cf4 molecules. *Phys. Rev. A*, **75**(6), 062714.
- 367.** Gualtieri, P., Picano, F., Casciola, C. M., & Piva, R. (2007). *Eddy viscosity and similarity models in les of shear flows*. XVIII Congresso AIMETA, 11-14 Settembre, 2007.
- 368.** Gualtieri, P., & Meneveau, C. (2007). *Numerical simulations of turbulence subjected to a straining and de-straining cycle*. 60th Annual Meeting of the Divison of Fluid Dynamics, November 18-20, 2007.
- 369.** Gualtieri, P., Casciola, C. M., Benzi, R., & Piva, R. (2007). Preservation of statistical properties in large-eddy simulation of shear turbulence. *J. Fluid Mech.*, **592**, 471-494.
- 370.** Hayakawa, K., Hatada, K., Della Longa, S., D'Angelo, P., & Benfatto, M. (2007). Progresses in the mxan fitting procedure. *AIP Conf. Proc.*, **882**, 111-113.
- 371.** Hernandez, E. R., Antonelli, A., Colombo, L., & Ordejon, P. (2007). *The calculation of free-energies in semiconductors: defects, transitions and phase diagrams* (Vol. 104).
- 372.** Ippolito, M., Mattoni, A., & Pugno, N. (2007). Failure strength of brittle materials containing nanovoids. *Phys. Rev. B*, **75**(22), 224110.
- 373.** Leggio, C., Anselmi, M., Di Nola, A., Galantini, L., Jover, A., Meijide, F., et al. (2007). Study on the structure of host-guest supramolecular polymers. *Macromolecules*, **40**(16), 5899-5906.
- 374.** Leonardi, S., Orlandi, P., & Antonia, R. A. (2007). *Heat transfer in a turbulent channel flow with roughness*. TSFP -5 5th International Symposium on Turbulence and Shear Flow Phenomena, August 27-29, 2007.
- 375.** Leonardi, S., Orlandi, P., & Antonia, R. A. (2007). Properties of d- and k-type roughness in a turbulent channel flow. *Phys. Fluids*, **19**(12), 125101.
- 376.** Leonardi, S., Castro, I. P., & Orlandi, P. (2007). *Turbulent flow over different groups of cubical obstacles* (Vol. 117) Springer Berlin-Heidelberg.
- 377.** Lundberg, D., Ullstrom, A. S., D'Angelo, P., & Persson, I. (2007). A structural study of the hydrated and the dimethylsulfoxide, n,n'-dimethylpropyleneurea, and n,n-dimethylthioformaraide solvated iron(ii) and iron(iii) ions in solution and solid state. *Inorg. Chim. Acta*, **360**(6), 1809-1818.

- 378.** Lundberg, D., Eriksson, L., D'Angelo, P., & Persson, I. (2007). A structural study of the n,n'-dimethylpropyleneurea solvated zinc(ii) and cadmium(ii) ions in solution and crystalline state. *J. Mol. Liq.*, **131-132**(Sp. Iss.), 105-112.
- 379.** Lundberg, D., Ullstrom, A. S., D'Angelo, P., Warminska, D., & Persson, I. (2007). On the complex formation of iron(iii) bromide in the space-demanding solvent n,n'-dimethylpropyleneurea and the structure of the trisbromoiron(iii) complex in solution and crystalline state. *Inorg. Chim. Acta*, **360**(8), 2744-2750.
- 380.** Marinetti, F., Coccia, E., Bodo, E., Gianturco, F. A., Yurtsever, E., Yurtsever, M., & Yildrim, E. (2007). Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures. *Theor. Chem. Acc.*, **118**(1), 53-65.
- 381.** Marinetti, F., Bodo, E., & Gianturco, F. A. (2007). Microsolvation of an ionic dopant in small he-4 clusters: oh+((3)sigma)(he-4)(n) via genetic algorithm optimizations. *ChemPhysChem*, **8**(1), 93-100.
- 382.** Masi, S., Ade, P. A. R., Bock, J. J., Bond, J. R., Borrill, J., Boscaleri, A., et al. (2007). The millimeter sky as seen with boomerang. *New Astron. Rev.*, **51**(3-4), 236-243.
- 383.** Matassa, R., Ballirano, P., Donzello, M., Ercolani, C., Sadun, C., & Caminiti, R. (2007). A nanostructured polymorph of muoxobis(phthalocyaninatoiron(iii)) studied by angular and energy dispersive x-ray diffraction. *Nano*, **2**(2), 121-128.
- 384.** Matassa, R., Sadun, C., D'Illario, L., Martinelli, A., & Caminiti, R. (2007). Supramolecular organization of toluidine blue dye in solid amorphous phases. *J. Phys. Chem. B*, **111**(8), 1994-1999.
- 385.** Matassa, R., Carbone, M., Lauceri, R., Purrello, R., & Caminiti, R. (2007). Supramolecular structure of extrinsically chiral porphyrin hetero-assemblies and achiral analogues. *Adv. Mater.*, **19**(22), 3961-3967.
- 386.** Mattoni, A., Ippolito, M., & Colombo, L. (2007). Atomistic modeling of brittleness in covalent materials. *Phys. Rev. B*, **76**(22), 224103.
- 387.** Meloni, S., Rosati, M., & Colombo, L. (2007). Efficient particle labeling in atomistic simulations. *J. Chem. Phys.*, **126**(12), 121102.
- 388.** Muscari, R., Broglia, R., & Di Mascio, A. (2007). Numerical simulation of the flow around an array of free-surface piercing cylinders in waves. *Ship. Tech. Res.*, **54**, 43-52.
- 389.** Orlandi, P., Leonardi, S., & Amati, G. (2007). *Dns of conjugate heat transfer in turbulent channel flows*. TSFP-5 5th International Symposium on Turbulence and Shear Flow Phenomena, August 27-29, 2007.
- 390.** Persson, I., Risberg, E. D., D'Angelo, P., De Panfilis, S., Sandstrom, M., & Abbasi, A. (2007). X-ray absorption fine structure spectroscopic studies of octakis(dimethyl sulfoxide)lanthanoid(iii) complexes in solution and in the solid iodides. *Inorg. Chem.*, **46**, 7742-7748.
- 391.** Piacentini, F., Ade, P. A. R., Bock, J. J., Bond, J. R., Borrill, J., Boscaleri, A., et al. (2007). Cmb polarization with boomerang 2003. *New Astron. Rev.*, **51**(3-4), 244-249.
- 392.** Picano, F., & Casciola, C. M. (2007). Small-scale isotropy and universality of axisymmetric jets. *Phys. Fluids*, **19**(11), 118106.
- 393.** Pirozzoli, S., Bernardini, M., & Grasso, F. (2007). *Aeroacoustics of transonic shock-boundary layer interactions*. 13th AIAA/CEAS Aeroacoustics Conference (28th AIAA Aeroacoustics Conference), May 21-23, 2007.
- 394.** Pirozzoli, S., Bernardini, M., & Grasso, F. (2007). Characterization of coherent vortical structures in a supersonic turbulent boundary layer. *J. Fluid. Mech.*, **613**, 205-231.
- 395.** Piva, R., Casciola, C. M., & De Angelis, E. (2007). *Turbulence of drug-reducing polymer solutions*. 11th EUROMECH European Turbulence Conference, June 25-28, 2007.
- 396.** Pizzitutti, F., Marchi, M., & Sterpone, F. (2007). How protein surfaces induce anomalous dynamics of hydration water. *J. Phys. Chem. B*, **111**(26), 7584-7590.
- 397.** Pugno, N., Carpinteri, A., Ippolito, M., Mattoni, A., & Colombo, L. (2007). Atomistic fracture: qfm vs md. *Eng. Fract. Mech.*, **75**, 1794-1803.
- 398.** Ramondo, F., Bencivenni, L., Caminiti, R., Pieretti, A., & Gontrani, L. (2007). Dimerisation of urea in water solution: a quantum mechanical investigation. *Phys. Chem. Chem. Phys.*, **9**(18), 2206-2215.
- 399.** Sanna, N., Castrignanò, T., D'Onorio De Meo, P., Carrabino, D., Grandi, A., Morelli, G., et al. (2007). Gaussian grid: a computational chemistry experiment over a web service-oriented grid. *Theor. Chem. Acc.*, **117**(5-6), 1145-1152.
- 400.** Sannino, G., Carillo, A., & Artale, V. (2007). Three-layer view of transports and hydraulics in the strait of gibraltar: a three-dimensional model study. *J. Geophys. Res.*, **112**, C03010.
- 401.** Santonico, E., Panni, S., Falconi, M., Castagnoli, L., & Cesareni, G. (2007). Binding to dpf-motif by the pob1 eh domain is responsible for pob1-eps15 interaction. *BMC Biochemistry*, **8**(1), 29.
- 402.** Scarel, G., Debernardi, A., & Tsoutsou, D. (2007). Vibrational and electrical properties of hexagonal la₂o₃ films. *Appl. Phys. Lett.*, **91**(10), 102901.
- 403.** Tacconi, M., Bodo, E., & Gianturco, F. A. (2007). Interaction of nh(x3sigma-) with rb and cs atoms: similarities and differences from an highly correlated ab initio study. *Theor. Chem. Acc.*, **117**(5-6), 649-662.
- 404.** Tacconi, M., Bodo, E., & Gianturco, F. A. (2007). Sympathetic cooling of nh (x3 sigma-) molecules by rb and cs atoms at ultralow energies. *Phys. Rev. A*, **75**(1), 012708.

- 405.** Valentini, A., Biancolella, M., Amati, F., Gravina, P., Miano, R., Chillemi, G., *et al.* (2007). Valproic acid induces neuroendocrine differentiation and UGT2B7 up-regulation in human prostate carcinoma cell line. *Drug. Metab. Dispos.*, **35**(6), 968-972.
- 406.** Yurtsever, E., Yildrim, E., Yurtsever, M., Bodo, E., & Gianturco, F. A. (2007). Solvation of k⁺ in helium droplets. *Eur. Phys. J. D.*, **43**(1-3), 105-108.
- 407.** Zazza, C., & Bencivenni, L. (2007). A dft study on the low-lying excited states and adiabatic photo-dissociation channels of nitric acid. *Internet Electron. J. Mol. Des.*, **6**(3), 70-80.
- 408.** Zazza, C., Meloni, S., Palma, A., Knupfer, M., Fuentes, G. G., & Car, R. (2007). Quasi-one-dimensional k-o chain in ptcda thin films: evidence from first-principles calculations. *Phys. Rev. Lett.*, **98**(4), 046401.
- 409.** Zazza, C., Sanna, N., & Aschi, M. (2007). Theoretical Study of alpha-84 Phycocyanobilin Chromophore from the Thermophilic Cyanobacterium Synechococcus elongatus. *J. Phys. Chem. B*, **111**(20), 5596-5601.
- 410.** Zollo, G., & Leahu, G. (2007). Electrical and optical characterization of a zn-implanted inp laser annealed in a nitrogen atmosphere. *Semicond. Sci. Technol.*, **22**, 292-297.
- 411.** Zollo, G., & Gala, F. (2007). Stability of i3 complexes in iii-v compound semiconductors by tight-binding molecular dynamics. *Phys. Rev. B*, **75**, 115205.
- 412.** Delugas, P., Fiorentini, V., Filippetti, A., & Pourtois, G. (2007). *First-principles calculation of high-k dielectric materials*. Kerala, India: Transworld Research Network.
- 413.** Palla, P., Ippolito, M., Giordano, S., Mattoni, A., & Colombo, L. (2007). *Atomistic approach to nanomechanics: concepts, methods, and (some) applications*. Kerala, India: Transworld Research Network.