

GFMUL

PUBLICATIONS IN 2003/2004

THESIS

1. GUEDES, R.C. - « Solvatação diferencial do fenol e do radical fenoxilo: Microsolvatação e simulação Monte Carlo », Ph.D. Dissertation, co-supervisors: Benedito J.C. Cabral, José Artur Martinho Simões, Universidade de Lisboa, Portugal, 2003.

BOOK (AUTHOR)

1. CHUNG, K.L. ; ZAMBRINI, J.C. - « Introduction to Random Time and Quantum Randomness », Monographs of the Portuguese Mathematical Society, 2nd edition, World Scientific, 2003, 211 pages. ISBN: 981-238-415-4

BOOK (EDITOR)

1. REBOLLEDO, R. ; REZENDE, J. ; ZAMBRINI, J.-C. - « Stochastic Analysis and Mathematical Physics », Proceedings of the International Symposium « The mathematical legacy of Feynman's path integral approach : Analysis, Geometry and Probability » (Lisbon, Portugal, June 2002), World Scientific, 2004.

CHAPTERS IN BOOKS

1. CANUTO, S. ; COUTINHO, K. ; COSTA CABRAL, B.J. - « Hydrogen Bonding and the Energetics of Homolytic Bond Dissociation in Solution: a Sequential Monte Carlo/Quantum Mechanics Approach », Invited Chapter to be published in Fundamental World of Quantum Chemistry. A Tribute to Per-Olov Löwdin, Vol. III. Editors: E.J. Brändas, E.S. Kryachko, Kluwer.

COMMUNICATIONS IN PROCEEDINGS

1. COUTINHO, R. ; FERNANDEZ, B. - « Iterative construction of fronts in bistable extended systems », Iteration Theory – ECIT'02 (Proceedings of the 14th International Conference on Iteration Theory, Évora, Portugal, September 2002), Eds: J. Sousa Ramos, D. Gronau, C. Mira, L. Reich, A. Sharkovsky, Grazer Math. Ber., Bericht Nr. 346 (2004), 91-97. ISSN 1016-7692
2. CRUZEIRO, A.B. ; XIANG, K.-N. - « On metrics for tangent processes on the path space », Stochastic Analysis and Related Topics VIII (Proceedings of the Silivri Workshop in Gazimagusa, North Cyprus, September, 2000), Eds: U. Capar and A.S. Ustunel, Progress in Probability, Birkhäuser, nº53, 2003.
3. CRUZEIRO, A.B. ; ZHANG, X. - « A Littlewood-Paley type inequality on the path space », Proceedings of the Seminar on Stochastic Analysis, Random Fields and Applications IV

(Ascona, Switzerland, May 2002), Eds. R. Dalang et al., Progress in Probability, Birkhäuser, n°58, 2004.

4. CRUZEIRO, A.B. - « Non adapted transformations of the Wiener measure », Stochastic Analysis and Mathematical Physics (Proceedings of the International Symposium « The mathematical legacy of Feynman's path integral approach : Analysis, Geometry and Probability », Lisbon, Portugal, June 2002), Eds. R. Rebolledo, J. Rezende, J.-C. Zambrini, World Scientific, 2004.
5. CRUZEIRO, A.B. ; ZHANG, X. - « Ornstein-Uhlenbeck semigroups on Riemannian path spaces », to be published in Proceedings of the First Sino-German Conference on Stochastic Analysis (Beijing, China, 2002), Eds. S. Albeverio, Z.M. Ma, M. Röckner, Science Press.
6. LESCOT, P. ; ZAMBRINI, J.C. - « Isoectors for the Hamilton-Jacobi-Bellman equation, formal stochastic differentials and first integrals in Euclidean Quantum Mechanics », Proceedings of the Seminar on Stochastic Analysis, Random Fields and Applications IV (Ascona, Switzerland, May 2002), Eds. R. Dalang et al., Progress in Probability, Birkhäuser, n°58, 2004.

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1. ARAÚJO, T. ; LOUÇÃ, F. ; MENDES, R.V. - « Reconstructing an economic space from a market metric », Physica A 323 (2003), 635.
2. ARAÚJO, T. ; SEIXAS, J.; MENDES, R.V. - « Dynamical characterization of the small-world phase », Physics Letters A 319 (2003), 285-289.
3. BRANCO, P. ; DENTE, J. ; MENDES, R.V. - « Using immunology principles for anomaly detection in electrical systems », IEEE Transactions in Industrial Electronics 50 (2003), 362-373.
4. CABRAL DO COUTO, P. ; GUEDES, R.C. ; COSTA CABRAL, B.J. - « The density of states and band gap of liquid water by sequential Monte Carlo/Quantum mechanics calculations », Brazilian Journal of Physics (Special Issue), 34 (1) (2004), 42-47.
5. CABRAL DO COUTO, P. ; GUEDES, R.C. ; COSTA CABRAL, B.J. ; MARTINHO SIMÕES, J.A. - « The hydration of the OH radical: microsolvation modeling and statistical mechanics simulation », Journal of Chemical Physics 119 (2003), 7344-7356.
6. CARLEN, E.A.; CARVALHO, M.C.; ESPOSITO, R.; LEBOWITZ, J.; MARRA, R. - « Free energy minimizers for a two-species model with segregation and liquid-vapour transition », Nonlinearity 16 (3) (2003), 1075-1105.
7. CARLEN, E.A.; CARVALHO, M.C.; LOSS, M. - « Spectral Gap for the Kac Model and Related Stochastic Evolutions », Acta Mathematica 191 (2003).
8. CORREIA, C.F. ; GUEDES, R.C. ; BORGES DOS SANTOS, R.M. ; COSTA CABRAL, B.J.; MARTINHO SIMÕES, J.A. - « O-H bond dissociation enthalpies in hydroxyphenols. A time-resolved photoacoustic calorimetry and quantum chemistry study », Physical Chemistry Chemical Physics, 6 (2004), 2109-2118.

9. CORREIA, C.F. ; BORGES DOS SANTOS, R.M. ; ESTÁCIO, S.G. ; COSTA CABRAL, B.J. ; MARTINHO SIMÕES, J.A. - « Reaction of Para-Hydroxyl-Substituted Diphenylmethane with Tert-Butoxy Radical », *ChemPhysChem*, 5 (2004), 1217-1221.
10. COUTINHO, Kaline ; GUEDES, R.C. ; COSTA CABRAL, B.J. ; CANUTO, Sylvio - « Electronic polarization of liquid water : convergent Monte-Carlo results for the multipole moments », *Chemical Physics Letters* 369 (2003), 345-353.
11. COUTINHO, R ; FERNANDEZ, B. - « Fronts in extended systems of bistable maps coupled via convolutions », *Nonlinearity*, 17 (2004), 23-47.
12. COUTINHO, R.; FERNANDEZ, B. - « Spatially extended circle maps: Monotone periodic dynamics of functions with linear growth », *Journal of Nonlinear Science*, 14 (2004), 93-118.
13. CRUZEIRO, A.B. ; MALLIAVIN, P. ; THALMAIER, A. - « Geometrization of Monte-Carlo numerical analysis of an elliptic operator : strong approximation », *C.R. Acad. Sci., Ser. I*, 338 (2004), p. 481-486.
14. CRUZEIRO, A.B. ; ZHANG, X. - « Finite dimensional approximation of Riemannian path space geometry », *J. Funct. Anal.* 205 (2003), 206-270.
15. ESTÁCIO, S.G. ; CABRAL DO COUTO, P. ; GUEDES, R.C. ; COSTA CABRAL, B.J. ; MARTINHO SIMÕES, J.A. - « Homolytic dissociation in hydrogen bonding liquids: energetics of phenol O-H bond in methanol and water and water O-H bond in water », *Theoretical Chemical Accounts*, 112 (2004), 282-289.
16. GODINHO, S.S.M.C. ; ROYO, Beatriz ; LOBATO, Maria T. ; HERDTWECK, Eberhardt ; ROMÃO, C.C. - « Synthesis and Structure of Diphenylphosphine Derivatives of Molybdenocene », *Polyhedron*, 23 (2004), 1263-1270.
17. GUEDES, R.C. ; CABRAL DO COUTO, P. ; COSTA CABRAL, B.J. - « Binding energy, structure and vibrational spectra of (HCl)₂₋₆ and (HF)₂₋₁₀ clusters by density functional theory », *Journal of Chemical Physics* 118 (3) (2003), 1272-1281.
18. GUEDES, R.C. ; COUTINHO, Kaline ; COSTA CABRAL, B.J. ; CANUTO, Sylvio - « Differential hydration of phenol and phenoxy radical and the energetics of the phenol O-H bond in solution », *Journal of Physical Chemistry B* 107 (2003), 4304-4310.
19. GUEDES, R.C. ; COUTINHO, Kaline ; COSTA CABRAL, B.J. ; CANUTO, Sylvio ; CORREIA, C.F. ; BORGES DOS SANTOS, R.M. ; MARTINHO SIMÕES, J.A. - « Solvent effects on the energetics of the phenol O-H bond : differential solvation of phenol and phenoxy radical in benzene and acetonitrile », *Journal of Physical Chemistry A*, 107 (2003), 9197-9207.
20. KARWOWSKI, W. ; MENDES, R.V. - « Quantum control in infinite dimensions », *Physics Letters A*, 322 (5-6) (2004), 282-285.
21. KONDRATIEV, Yu. G. ; KUNA, T. ; OLIVEIRA, M.J. - « On the relations between Poissonian white noise analysis and harmonic analysis on configuration spaces », *J. Funct. Anal.* 213 (1) (2004), 1-30.
22. LOPES, S.C.D.N. ; GOORMAGHTIGH, E. ; COSTA CABRAL, B.J. ; CASTANHO.

M.A.R.B. - « Filipin Orientation Revealed by Linear Dichroism. Implication for a Model of Action. », *Journal of the American Chemical Society*, 126 (2004), 5396-5402.

23. MAN'KO, V.I. ; MENDES, R.V. - « Quantum control and the Strocchi map », *Physical Review A* 67 (2003), 053404.
24. MATA, R.A. ; COSTA CABRAL, B.J. - « Energetics, Structure, and Electronic Properties of (CH₃CN)₂₋₈ Clusters by Density Functional Theory », *Journal of Molecular Structure (Theochem)*, 673 (2004), 155-164.
25. MENDES, R.V. - « Network dependence of strong reciprocity », *Advances in Complex Systems*, 7 (2004), 1-12.
26. MENDES, R.V. - « Quantum collision states for positive charges in an octahedral cage », *International Journal of Hydrogen Energy* 28 (2003), 125.
27. MENDES, R.V. - « Stratification of the orbit space in gauge theories. The role of nongeneric strata. », *J. Phys. A : Math. Gen.* 37 (2004), 1-14.
28. MENDES, R.V. - « The nonlinear directional coupler. An analytic solution », *Optics Communications*, 232 (2004), 425-427.
29. MENDES, R.V. ; VAZQUEZ, L. - « Fractionally coupled solutions of the diffusion equation », *Applied Mathematics and Computation* 141 (2003), 125-130.
30. PRIVAULT, N. ; ZAMBRINI, J.C. - « Markovian bridges and reversible diffusion processes with jumps », *Annales de l'Institut Henri Poincaré (Probabilités & Statistiques)*, 40 (2004), 599-633.

PAPERS ACCEPTED FOR PUBLICATION

1. COSTA CABRAL, B.J. - « The Vibrational Structure of the OH Radical in Solid Argon: a Transfer-Matrix Path-Integral Approach », to be published in *International Journal of Quantum Chemistry*.
2. COUTINHO, K. ; COSTA CABRAL, B.J. ; CANUTO, S. - « Can larger dipoles solvate less ? Solute-Solvent hydrogen bond and the differential solvation of phenol and phenoxy », to be published in *Chem. Phys. Lett.*
3. CRUZEIRO, A.B. ; ZHANG, X. - « L^p-gradient estimates of symmetric Markov semigroups for 1<p≤2 », to be published in *Acta Math. Sinica*.
4. ESTÁCIO, S.G. ; CABRAL DO COUTO, P. ; COSTA CABRAL, B.J. ; MINAS DA PIEDADE, M. E. ; MARTINHO SIMÕES, J. A. - « Energetics of Intramolecular Hydrogen Bonding in Di-substituted benzenes by the ortho-para Method », to be published in *J. Phys. Chem. A*.
5. GODINHO, S.S.M.C. ; CABRAL DO COUTO, P. ; COSTA CABRAL, B.J. - « Charge separation and charge transfer to solvent (CTTS) in NaCl-water clusters », to be published in *Chem. Phys. Lett.*

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7. MENDES, R.V. - « Tools for network dynamics », to be published in Int. Journal of Bifurcation and Chaos.
8. PRIVAULT, N. ; ZAMBRINI, J.C. - « Euclidean quantum mechanics in the momentum representation », to be published in Journal of Mathematical Physics.