

RESEARCH GROUP: MOLECULAR DYNAMICS OF COMPLEX SYSTEMS

Publications in peer review Journals

1. C.E.S. Bernardes, M.E.M. da Piedade, L.M.P.F. Amaral, et al. - Energetics of C-F, C-Cl, C-Br, and C-I bonds in 2-haloethanols. Enthalpies of formation of $\text{XCH}_2\text{CH}_2\text{OH}$ ($\text{X}=\text{F}, \text{Cl}, \text{Br}, \text{I}$) compounds and of the 2-hydroxyethyl radical. *Journal of Physical Chemistry A* 111 (9) (2007), 1713-1720.
2. F. Agapito, B.J.C. Cabral, J.A.M. Simões - A cost-effective basis-set extrapolation scheme: Application to the energetics of homolytic bond dissociation, *Journal of Molecular Structure-Theochem* 811 (1-3) (2007), 361-372.
3. F. Agapito, P.M. Nunes, B.J.C. Cabral et al. - Energetics of the allyl group, *Journal of Organic Chemistry* 72 (23) (2007), 8770-8779.
4. H.F.M.C. Martiniano, B.J.C. Cabral, J.A. Simões - Substituent effects on water-assisted proton transfer in [$\text{p-XC}_6\text{H}_4\text{OH-(H}_2\text{O)(1-3)}$] $(\cdot+)$ clusters, *Chemical Physics Letters* 442 (4-6) (2007), 451-459.
5. M.P.S. Mateus, B.J.C. Cabral - Electron binding energies of organic azides: Green's function and density functional theory versus Hartree-Fock calculations, *Chemical Physics Letters* 448 (4-6) (2007), 280-286.
6. N. Couto, M.F. Duarte, M.T. Fernandez et al. - Complexation of transition metals by 3-azidopropionitrile. An electrospray ionization mass spectrometry study. *Journal of the American Society for Mass Spectrometry* 18 (3) (2007), 453-465.
7. N. Galamba, B.J.C. Cabral - First principles molecular dynamics of molten NaI: Structure, self-diffusion, polarization effects, and charge transfer, *Journal of Chemical Physics* 127 (9) (2007), 094506.
8. N. Galamba, B.J.C. Cabral - First principles molecular dynamics of molten NaCl, *Journal of Chemical Physics* 126 (12) (2007), 124502.
9. P.C. do Couto, B.J.C. Cabral - Electronically excited water aggregates and the adiabatic band gap of water, *Journal of Chemical Physics* 126 (1) (2007), 014509.
10. R.M. Borges dos Santos, B.J. Costa Cabral, J.A. Martinho Simões - Bond-dissociation enthalpies in the gas phase and in organic solvents: Making ends meet, *Pure and Applied Chemistry* 79 (8) (2007), 1369-1382.

RESEARCH GROUP: ANALYSIS AND GEOMETRY IN MATHEMATICAL PHYSICS

Publications in peer review Journals

1. N. Manojlovic, Z. Nagy - Algebraic Bethe ansatz for the elliptic quantum group $E\text{-}\tau, E\text{-}\eta(A(2)((2)))$. *J. Math. Phys.* Vol.48, No. 12 (2007), 123515, 11 pages.
2. N. Manojlovic, Z. Nagy - Creation operators and algebraic Bethe ansatz for the elliptic quantum group $E\text{-}\tau, E\text{-}\eta(so(3))$. *J. Phys. A: Math. Theor.* 40 (2007), 4181-4191.
3. N.C. Dias, J.N. Prata - Deformation Quantization of Confined Systems. *Int. J. Quantum Inf.* 5 (2007), 257.
4. N.C. Dias, J.N. Prata - Environment-Induced Decoherence in Noncommutative Quantum Mechanics. *Int. J. Quantum Inf.* 5 (2007), 287.
5. N.C. Dias, J.N. Prata - Features of Moyal trajectories. *J. Math. Phys.* 48 (2007), 012109, 23 pages.
6. P. Freitas - Precise bounds and asymptotics for the first Dirichlet eigenvalue of triangles and rhombi. *J. Funct. Anal.* 251 (2007), 376-398.
7. P. Freitas, D. Krejcirk - Unbounded planar domains whose second nodal line does not touch the boundary. *Math. Res. Lett.* 14 (2007), 107-111.
8. P. Freitas, R.S. Laugesen, G.F. Liddell - On convex surfaces with minimal moment of inertia. *J. Math. Phys.* 48 (2007), 122902, 21 pages.

Other Publications

(Include books, chapters or full papers published in conference proceedings)

1. A. Mikovic - Graviton Propagator from Spin Networks. Proceedings of the 4-th Summer School in Modern Mathematical Physics, 3-14 September 2006, Belgrade (Institute of Physics, Belgrade 2007).
2. A. Bastos, O. Bertolami, N.C. Dias, J.N. Prata - Deformation quantization of noncommutative quantum mechanics and dissipation. *Journal of Physics: Conference Series* 67 (2007), 012058.
3. N. Manojlovic, Z. Nagy - Construction of the Bethe state for the $E\text{-}\tau, E\text{-}\eta(so(3))$ elliptic quantum group. *SIGMA* 3 (2007), 004, 10 pages.
4. P.P. Kulish, N. Manojlovic - Quantum algebras with representation ring of sl_2 type. *Zapiski Nauchnyh Seminarov POMI* 347 (2007), 167-177.

RESEARCH GROUP: STOCHASTIC ANALYSIS, PATH INTEGRALS AND APPLICATIONS

Publications in peer review Journals

1. A.B. Cruzeiro, F. Flandoli, P. Malliavin - Brownian motion on volume preserving diffeomorphisms group and existence of global solutions of 2D stochastic Euler equation. *J. Funct. Anal.* 242 (1) (2007), 304-326.
2. F. Cipriano, A.B. Cruzeiro - Navier-Stokes Equation and Diffusions on the group of Homeomorphisms of the torus. *Comm. Math. Phys.* 275 (2) (2007), 255-269.
3. S. Chaari, F. Cipriano, H. Ouerdiane - Large deviation properties of solutions of nonlinear stochastic convolution equations. *Adv. Theor. Appl. Math.* 2 (1) (2007), 1-14.

Other Publications

(Include books, chapters or full papers published in conference proceedings)

1. A.B. Cruzeiro, H. Ouerdiane, N. Obata - Mathematical Analysis of Random Phenomena (Proceedings of the International Conference, Hammamet, Tunisia, 12-17 September 2005), World Scientific, 2007.
2. J.C. Zambrini, J.C. Mourão, J.P. Nunes, R. Picken – Prospects in Mathematical Physics, Contemporary Mathematics 437, American Mathematical Society, 2007.
3. A.B. Cruzeiro, P. Malliavin - Stochastic evolution of inviscid Burgers fluid, in Probability, Geometry and Integrable Systems, MSRI Publications, Vol. 55, 2007.
4. F. Cipriano, A.B. Cruzeiro - Variational principle for diffusions on the diffeomorphism group with the H^2 metric. Mathematical Analysis of Random Phenomena, 85-91, World Sci. Publ., Hackensack, NJ, 2007.
5. F. Cipriano, H. Ouerdiane, J.L. Silva, R. Vilela Mendes - Nonlinear stochastic equation of convolution type. Mathematical Analysis of Random Phenomena, 73-84, World Sci. Publ., Hackensack, NJ, 2007.
6. J.C. Zambrini - From the geometry of parabolic PDE to the geometry of stochastic differential equations. Mathematical Analysis of Random Phenomena, 213-230, World Sci. Publ., Hackensack, NJ, 2007.