

Peer-reviewed journal articles

1)-David Bishop's approach to vibrational dynamic contributions to molecular properties.

Application to Jones and Magnetolectric birefringences in diatomic molecules

Rizzo, A.; Cappelli, C.

International journal of quantum chemistry 111 (2011): 760–771.

<https://dx.doi.org/10.1002/qua.22813>

2)-Cavity field effects within a polarizable continuum model of solvation: application to the calculation of electronic circular dichroism spectra of R-(+)-3-Methyl-cyclopentanone

Pipolo, S.; Cammi, R.; Rizzo, A.; Cappelli, C.; Mennucci, B.; Tomasi, J.

International journal of quantum chemistry 111 (2011): 826–838.

<http://www.cnr.it/prodotto/i/40327>

info:cnr-pdr/source/autori:Pipolo, S.; Cammi, R.; Rizzo, A.; Cappelli, C.; Mennucci, B.; Tomasi, J./titolo:Cavity field effects within a polarizable continuum model of solvation: application to the calculation of electronic circular dichroism spectra of R-(+)-3-Methyl-cyclopentanone/

3)-Size-dependent selectivity and activity of silver nanoclusters in the partial oxidation of propylene to propylene oxide and acrolein: A joint experimental and theoretical study

Molina L. M.; Lee S.; Sell K.; Barcaro G.; Fortunelli A.; Lee B.; Seifert S.; Winans R. E.; Elam J. W.; Pellin M. J.; Barke I.; von Oeynhausen V.; Lei Y.; Meyer R. J.; Alonso J. A.; Fraile-Rodriguez A.; Kleibert A.; Giorgio S.; Henry C. R.; et al.

Catalysis Today 160 (2011): 116–127.

<https://dx.doi.org/10.1016/j.cattod.2010.08.022>

4)-Structural properties of pulsed laser deposited SnOx thin films

Fazio E.; Neri F.; Ruggeri R.; Sabatino G.; Trusso S.; Mannino G.subjectTin oxidesubjectThin filmssubjectPulsed laser ablationsubjectTEM

Applied surface science 257 (2011): 2520–2525.

<http://www.cnr.it/prodotto/i/40389>

info:cnr-pdr/source/autori:Fazio E.; Neri F.; Ruggeri R.; Sabatino G.; Trusso S.; Mannino G./titolo:Structural properties of pulsed laser deposited SnOx thin films/

5)-Amphiphilic Amylose-g-poly(meth)acrylate Copolymers through “Click” onto Grafting Method

Bertoldo, Monica; Zampano, Giovanni; La Terra, Federico; Villari, Valentina; Castelvetro Valtersubjectamphiphilic graft copolymerssubjectamylosesubject“click” reactionsubjectpoly(meth)acrylatesubjectself-assembling

Biomacromolecules 12 (2011): 388–398.

<http://www.cnr.it/prodotto/i/40418>

info:cnr-pdr/source/autori:Bertoldo, Monica; Zampano, Giovanni; La Terra, Federico; Villari, Valentina; Castelvetro Valter/titolo:Amphiphilic Amylose-g-poly(meth)acrylate Copolymers through “Click” onto Grafting Method/

6)-Easy detectable isocyanate in the reaction with gelatin

Bertoldo, Monica; Cognigni, Federica; Ciardelli, Francesco/subjectGelatin/subjectIsocyanates/subjectUV–VIS spectroscopy/subjectFluorescence spectroscopy

Polymer bulletin (Berl., Print) (2011).

<http://www.cnr.it/prodotto/i/40419>

info:cnr-pdr/source/autori:Bertoldo, Monica; Cognigni, Federica; Ciardelli, Francesco/titolo:Easy detectable isocyanate in the reaction with gelatin/

7)-Raman scattering investigation of the boson peak in a sodium silicate glass

Baldi, Giacomo; Fontana, Aldo; Rossi, Flavio; Monaco, Giulio/subjectboson peaks/subjectglass/subjectelasticity

Philosophical magazine (2003, Print) 91 (2011): 1801–1808.

<https://dx.doi.org/10.1080/14786435.2010.523020>

8)-The Raman coupling function in permanently densified GeO₂ glasses

Orsingher, Laura; Baldi, Giacomo; Fontana, Aldo; Rossi, Flavio/subjectvitreous germania/subjectpermanently densified glass/subjectRaman light scattering/subjectneutron inelastic scattering

Philosophical magazine (2003, Print) 91 (2011): 1857–1863.

<https://dx.doi.org/10.1080/14786435.2010.527865>

9)-High frequency acoustic attenuation of vitreous silica: New insight from inelastic x-ray scattering

Baldi, Giacomo; Giordano, Valentina Maria; Monaco, Giulio; Ruta Beatrice/subjectSound attenuation; Vibrational dynamics; Glasses; Boson peak

Journal of non-crystalline solids 357 (2011): 538–541.

<https://dx.doi.org/10.1016/j.jnoncrysol.2010.05.085>

10)-The Johari–Goldstein beta-relaxation of glass-forming binary mixtures

Capaccioli, S.; Kessairi, K.; Shahin Thayyil, M.; Prevosto, D.; Lucchesi, M./subjectbinary mixtures/subjectstructural relaxations/subjectsecondary relaxations/subjectglass transition

Journal of non-crystalline solids 357 (2011): 251–257.

<http://www.cnr.it/prodotto/i/40596>

info:cnr-pdr/source/autori:Capaccioli, S.; Kessairi, K.; Shahin Thayyil, M.; Prevosto, D.; Lucchesi, M./titolo:The Johari–Goldstein beta-relaxation of glass-forming binary mixtures/

11)-Two-photon polarization dependent spectroscopy in chirality: A novel experimental-theoretical approach to study optically active systems.

Hernandez, F. E.; Rizzo, A. subjectChiralitysubjectNonlinear spectroscopysubjectTwo-photon processessubjectBinaphtolsubjectBy-aryls
Molecules (Basel, Online) 16 (2011): 3315–3337.
<https://dx.doi.org/10.3390/molecules16043315>

12)-Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals

Bast, R.; Ruud, K.; Rizzo, A.; Helkaker, T. subjectRelativistic effectssubjectBuckingham BirefringencesubjectNonlinear propertiessubjectResponse theory
Theoretical Chemistry accounts (Print) 129 (2011): 685–699.
<https://dx.doi.org/10.1007/s00214-011-0939-3>

13)-The particle distributions of asymmetric kinetic electrostatic structures

NOCERA L; PALUMBO L JsubjectBGK-modessubjectdouble-layerssubjectelectrostatic-solitary-wavessubjectphase-space-holessubjectsheaths
Physics of plasmas 18 (2011): 032114-1–032114-4.
<https://dx.doi.org/10.1063/1.3562875>

14)-Crystalline, mobile amorphous and rigid amorphous fractions in poly(L-lactic acid) by TMDSC

Righetti M.C.; Tombari E. subjectthree-phase modelsubjectcrystalline fractionssubjectrigid amorphous fractionssubjectmobile amorphous fractionssubjectchain mobility
522 (2011): 118–127.
<http://www.cnr.it/prodotto/i/40692>

info:cnr-pdr/source/autori:Righetti M.C., Tombari E./titolo:Crystalline, mobile amorphous and rigid amorphous fractions in poly(L-lactic acid) by TMDSC/

15)-Thermodynamic study of (heptane plus amine) mixtures. II Excess and partial molar volumes at 298.15 K

Lepori L.; Gianni P.; Spanedda A.; Matteoli E. subjectdensitysubjectexcess volumesubjectpartial molar volumesubjectheptanesubjectamine
Journal of Chemical Thermodynamics 43 (2011): 805–813.
<http://www.cnr.it/prodotto/i/40693>

info:cnr-pdr/source/autori:Lepori L., Gianni P., Spanedda A., Matteoli E./titolo:Thermodynamic study of (heptane plus amine) mixtures. II Excess and partial molar volumes at 298.15 K/

16)-The Influence of the Composition of an Aqueous-Acetone Solvent on the Thermodynamic Characteristic of Complex Formation of 18-Crown-6 Ether with Glycine

Usacheva T.R.; Kuz'mina I.A.; Sharnin V.A.; Chernov I.V.; Matteoli E. subjectbinary solventssubjectglycinesubjectcomplex formationsubjectthermodynamicssubjectenthalpy
Russian journal of physical chemistry 85 (2011): 948–951.
<http://www.cnr.it/prodotto/i/40694>

info:cnr-pdr/source/autori:Usacheva T.R., Kuz'mina I.A., Sharnin V.A., Chernov I.V., Matteoli E./titolo:The Influence of the Composition of an Aqueous-Acetone Solvent on the Thermodynamic Characteristic of Complex Formation of 18-Crown-6 Ether with Glycine/

17)-Thermodynamic study of heptane + secondary, tertiary and cyclic amines mixtures. Part IV. Excess and solvation enthalpies at 298.15 K

Matteoli E.; Gianni P.; Lepori L.subjectexcess enthalpysubjectmixturessubjectaminessubjectheptanesubjectsolvation

Fluid phase equilibria 306 (2011): 234–241.

<http://www.cnr.it/prodotto/i/40695>

info:cnr-pdr/source/autori:Matteoli E., Gianni P., Lepori L./titolo:Thermodynamic study of heptane + secondary, tertiary and cyclic amines mixtures. Part IV. Excess and solvation enthalpies at 298.15 K/

18)-Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K

Lepori L.; Gianni P.; Spanedda A.; Matteoli E.subjectdensitysubjectexcess volumesubjectpartial molar volumesubjectheptanesubjectamine

Journal of Chemical Thermodynamics 43 (2011): 1453–1462.

<http://www.cnr.it/prodotto/i/40696>

info:cnr-pdr/source/autori:Lepori L., Gianni P., Spanedda A., Matteoli E./titolo:Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K/

19)-Effect of Solvation on the Thermodynamics of the Formation of Molecular Complexes of 18Crown6 Ether with Glycine in Water–Dimethylsulfoxide Solutions

Usacheva T.R.; Sharnin V.A.; Matteoli E.

Russian journal of physical chemistry 85 (2011): 1989–1902.

<http://www.cnr.it/prodotto/i/40726>

info:cnr-pdr/source/autori:Usacheva T.R, Sharnin V.A., and Matteoli E./titolo:Effect of Solvation on the Thermodynamics of the Formation of Molecular Complexes of 18Crown6 Ether with Glycine in Water–Dimethylsulfoxide Solutions/

20)-Effect of Confinement on Structural Relaxation in Ultrathin Polymer Films Investigated by Local Dielectric Spectroscopy

Nguyen, H.; Prevosto, D.; Labardi, M.; Capaccioli, S.; Lucchesi, M.; Rolla, P.

Macromolecules (Print) 44 (2011): 6588.

<http://www.cnr.it/prodotto/i/40729>

info:cnr-pdr/source/autori:Nguyen, H.; Prevosto, D.; Labardi, M.; Capaccioli, S.; Lucchesi, M.; Rolla, P./titolo:Effect of Confinement on Structural Relaxation in Ultrathin Polymer Films Investigated by Local Dielectric Spectroscopy/

21)-Damped response theory description of two-photon absorption

Kristensen, K.; Kauczor, J.; Thorvaldsen, A. J.; Joergensen, P.; Kjaergaard, T.; Rizzo, A. *subjectDensity Functional TheorysubjectMolecule-Photon CollisionssubjectOrganic CompoundsubjectPhotoexcitationssubjectTwo-Photon Spectra*
The Journal of chemical physics 134 (2011): 214104.
<https://dx.doi.org/10.1063/1.3595280>

22)-The role of primitive relaxation in the dynamics of aqueous mixtures, nano-confined water and hydrated proteins

Capaccioli S.; Ngai K.L.; Ancherbak S.; Rolla P.A.; Shinyashiki N.
Journal of non-crystalline solids 357 (2011): 641–654.
<http://www.cnr.it/prodotto/i/40754>

info:cnr-pdr/source/autori:Capaccioli S., Ngai K.L., Ancherbak S., Rolla P.A., Shinyashiki N./titolo:The role of primitive relaxation in the dynamics of aqueous mixtures, nano-confined water and hydrated proteins/

23)-Resolving the ambiguity of the dynamics of water and clarifying its role in hydrated proteins

Ngai K.L.; Capaccioli S.; Ancherbak S.; Shinyashiki N.
91 (2011): 1809–1835.
<http://www.cnr.it/prodotto/i/40755>

info:cnr-pdr/source/autori:Ngai K.L., Capaccioli S., Ancherbak S., Shinyashiki N./titolo:Resolving the ambiguity of the dynamics of water and clarifying its role in hydrated proteins/

24)-Temperature and pressure dependence of secondary process in an epoxy system

Sharifi S.; Capaccioli S.; Lucchesi M.; Rolla P.A.; Prevosto; D.
134 (2011): 044510.
<http://www.cnr.it/prodotto/i/40756>

info:cnr-pdr/source/autori:Sharifi S., Capaccioli S., Lucchesi M., Rolla P.A., Prevosto, D./titolo:Temperature and pressure dependence of secondary process in an epoxy system/

25)-Resolving the controversy on the glass transition temperature of water?

Capaccioli; S.; Ngai; K.L.
135 (2011): 104504.
<http://www.cnr.it/prodotto/i/40757>

info:cnr-pdr/source/autori:Capaccioli, S., Ngai, K.L./titolo:Resolving the controversy on the glass transition temperature of water?/

26)-Structure of Ag-Pd nanoclusters adsorbed on MgO(100): A computational study

Negreiros F. R.; Barcaro G.; Kuntova Z.; Rossi G.; Ferrando R.; Fortunelli A.
Surface science 605 (2011): 483–488.
<https://dx.doi.org/10.1016/j.susc.2010.12.002>

27)-Structures of small Au clusters on MgO(001): a computational study

Ferrando R.; Barcaro G.; Fortunelli A.

Physical review. B, Condensed matter and materials physics 83 (2011): 045418.

<https://dx.doi.org/10.1103/PhysRevB.83.045418>

28)-Patchy Multishell Segregation in Pd-Pt Alloy Nanoparticles

Barcaro G.; Fortunelli A.; Polak M.; Rubinovich L.

Nano letters (Print) 11 (2011): 1766–1769.

<https://dx.doi.org/10.1021/nl200322s>

29)-Template-assisted assembly of transition metal nanoparticles on oxide ultrathin films

Gavioli L.; Cavaliere E.; Agnoli S.; Barcaro G.; Fortunelli A.; Granozzi G.

Progress in surface Science (Print) 86 (2011): 59–81.

<https://dx.doi.org/10.1016/j.progsurf.2011.02.001>

30)-Optical Properties of Au Nanoclusters from TD-DFT Calculations

Durante N.; Fortunelli A.; Broyer M.; Stener M.

Journal of physical chemistry. C 115 (2011): 6277–6282.

<https://dx.doi.org/10.1021/jp112217g>

31)-Optimization of chemical ordering in AgAu nanoalloys

Manuella Cerbelaud 1; 2; Riccardo Ferrando 1; 2; Giovanni Barcaro 3; Alessandro Fortunelli
3subjectELECTRONIC-STRUCTURESsubjectCHARGE EQUILIBRATIONsubjectGLOBAL
OPTIMIZATIONsubjectALLOY CLUSTERSsubjectAU NANOALLOYS

PCCP. Physical chemistry chemical physics (Print) 13 (2011): 10232–10240.

<https://dx.doi.org/10.1039/c0cp02845b>

32)-The two-dimensional cobalt oxide (9x2) phase on Pd(100)

Gragnaniello L.; Barcaro G.; Sementa L.; Allegretti F.; Parteder G.; Surnev S.; Steurer W.;
Fortunelli A.; Netzer F. P.

The Journal of chemical physics 134 (2011): 184706.

<https://dx.doi.org/10.1063/1.3578187>

33)-Homogeneous Nucleation of Graphitic Nanostructures from Carbon Chains on Ni(111)

Cheng D.; Barcaro G.; Charlier J.-C.; Hou M.; Fortunelli A.

Journal of physical chemistry. C 115 (2011): 10537–10543.

<https://dx.doi.org/10.1021/jp2028092>

34)-Interplay between layer-resolved chemical composition and electronic structure in a Sn/Pt(110) surface alloy

Agnoli S.; Barcaro G.; Barolo A.; Fortunelli A.; Sambì M.; Sedona F.; Di Marino M.; Skala T.; Granozzi G.

Journal of physical chemistry. C 115 (2011): 14264–14269.

<https://dx.doi.org/10.1021/jp2034278>

35)-Tracking thermally-activated transformations in a nanostructured metal/oxide/metal system

Cavaliere E.; Artiglia L.; Barcaro G.; Rizzi G. A.; Bondino F.; Fortunelli A.; Gavioli L.; Granozzi G.

PCCP. Physical chemistry chemical physics (Print) 13 (2011): 17171–17176.

<https://dx.doi.org/10.1039/C1CP22013F>

36)-Metamorphosis of ultrathin Ni oxide nanostructures on Ag(100)

Steurer W.; Allegretti F.; Surnev S.; Barcaro G.; Sementa L.; Negreiros F. R.; Fortunelli A.; Netzer F. P.

Physical review. B, Condensed matter and materials physics 84 (2011): 115446.

<https://dx.doi.org/10.1103/PhysRevB.84.115446>

37)-Differences in Two-photon and One-photon Absorption Profiles induced by Vibronic Coupling. The case of dioxaborine heterocyclic dye.

Lin, N.; Luo, Y.; Ruud, K.; Zhao, X.; Santoro, F.; Rizzo A. subjectab initio calculationssubjectdensity functional calculationssubjectlaser spectroscopysubjectnonlinear opticssubjectspectroscopic methods

ChemPhysChem (Print) 12 (2011): 3392–3403.

<https://dx.doi.org/10.1002/cphc.201100500>

38)-Computational prediction of selectivities in nonreversible and reversible hydroformylation reactions catalysed by unmodified rhodium catalysts

Giuliano Alagona; Raffaello Lazzaroni; Caterina Ghio subjectB3P86/6-31G*/LanL2DZsubjectHydroformylationsubjectregioselectivity

Journal of molecular modeling (Print) 17 (2011): 2275–2284.

<https://dx.doi.org/10.1007/s00894-010-0864-8>

39)-Scanning Electro-optic Microscopy of Ferroelectric Domain Structure with a Near-Field Fiber Probe

Tikhomirov O. [1]; Labardi M. [2]; Ascoli C. [3]; Allegrini M. [4,3] subjectOPTICAL MICROSCOPYsubjectTHIN-FILMSsubjectPHASE-TRANSITIONSsubjectPOLARIZATION

Journal of applied physics 110 (2011): 084117–084117.

<https://dx.doi.org/10.1063/1.3656731>

40)-Structure and bonding of tungsten oxide clusters on nanostructured Cu-O surfaces

Wagner M.; Surnev S.; Ramsey M. G.; Barcaro G.; Sementa L.; Negreiros F. R.; Fortunelli A.; Dohnalek Z.; Netzer F. P.

Journal of physical chemistry. C 115 (2011): 23480–23487.

<https://dx.doi.org/10.1021/jp208207e>

41)-Interface effects on the magnetism of CoPt supported nanostructures

Barcaro G.; Sementa L.; Negreiros F. R.; Ferrando R.; Fortunelli A.

Nano letters (Print) 11 (2011): 5542–5546.

<https://dx.doi.org/10.1021/nl203449y>

42)-Alloying effects on the optical properties of Ag-Au nanoclusters from TDDFT calculations

Barcaro G.; Broyer M.; Durante N.; Fortunelli A.; Stener M.subjectChimica computazionale

Journal of physical chemistry. C 115 (2011): 24085–24091.

<https://dx.doi.org/10.1021/jp2087219>

43)-Effective interactions between colloidal particles suspended in a bath of swimming cells

Angelani, L.; Maggi, C.; Bernardini, M.L.; Rizzo, A.; Di Leonardo, R.subjectColloidal particle; Colloidal suspensions; Colloidal tracers; Depletion force; Effective interactions; Excluded volume effects; Non-equilibrium dynamics; Nonequilibrium statistical mechanics; Self-propelled particles; Short-range attraction

Physical review letters (Print) 107 (2011): 138302.

<https://dx.doi.org/10.1103/PhysRevLett.107.138302>

44)-Ising M-p-spin mean-field model for the structural glass: Continuous versus discontinuous transition

Caltagirone, F.; Ferrari, U.; Leuzzi, L.; Parisi, G.; T. Rizzo, T.subjectPOTTS GLASS; TEMPERATURE-DEPENDENCE; METASTABLE STATES; PHASE-TRANSITION; FORMING LIQUIDS; DYNAMICS; RELAXATION; VISCOSITY; STATICS; SYMMETRY

Physical review. B, Condensed matter and materials physics (Online) 83 (2011): 104202.

<https://dx.doi.org/10.1103/PhysRevB.83.104202>

45)-Melting temperature evolution of non-reorganized crystals. Poly(3-hydroxybutyrate)

Righetti M.C.; Di Lorenzo M.L.subjectSuperheatingsubjectThermal lagsubjectReorganizationsubjectsuperheatingsubjectthermal lagsubjectreorganization

512 (2011): 59–66.

<http://www.cnr.it/prodotto/i/168983>

info:cnr-pdr/source/autori:Righetti M.C.; Di Lorenzo M.L./titolo:Melting temperature evolution of non-reorganized crystals. Poly(3-hydroxybutyrate)/

46)-Computational challenges in simulating and analyzing experimental linear and nonlinear circular dichroism spectra. R-(+)-1,1'-bi(2-naphthol) as a prototype case

Lin N.; Santoro F.; Zhao X.; Toro C.; De Boni L.; Hernandez F. E.; Rizzo A. subjecttwo-photons subjectcircular dichroism subjectBinaphthol subjectTD-DFT
The journal of physical chemistry. B 115 (2011): 811–824.
<https://dx.doi.org/10.1021/jp108669f>

47)-Structural properties of pulsed laser deposited SnO(x) thin films

Fazio E.; Neri F.; Ruggeri R.; Sabatino G.; Trusso S.; Mannino G.
Applied surface science 257 (2011): 2520–2525.
<http://www.cnr.it/prodotto/i/170879>

info:cnr-pdr/source/autori:Fazio E., Neri F., Ruggeri R., Sabatino G., Trusso S., Mannino G./titolo:Structural properties of pulsed laser deposited SnO(x) thin films/

48)-Compatible blends of biorelated polyesters through catalytic transesterification in the melt

Maria-Beatrice Coltelli a,b,*; Claudio Toncelli a; Francesco Ciardelli a,b; Simona Bronco
c subjectBiodegradable polyesters subjectReactive
blendings subjectTransesterifications subjectPoly(lactide) subjectPoly(butylene adipate-co-
terephthalate)
Polymer degradation and stability 96 (2011): 982–990.
<https://dx.doi.org/10.1016/j.polymdegradstab.2011.01.028>

49)-Colour responsive smart polymers and biopolymers films through nanodispersion of organic chromophores and metal particles

Andrea Pucci a,b,c, Giacomo Ruggeri a,c,d; Simona Bronco d,c; Francesca Signori d,c; Filippo Donati a; Marco Bernabò a; Francesco Ciardelli a,d,* subjectPolymers subjectFilms. Optical responses subjectSmart materials subjectStimulated light emission
Progress in organic coatings (Print) 72 (2011): 21–25.
<https://dx.doi.org/10.1016/j.porgcoat.2010.12.015>

50)-Radical functionalization of poly(butylene succinate-co-adipate): Effect of cinnamic co-agents on maleic anhydride grafting

Francesca Signori a,b,*; Marco Badalassi c; Simona Bronco a; Francesco Ciardelli
d subjectFunctional biodegradable polyesters subjectRadical graftings subjectMAH
graftings subjectcinnamic co-agent
Polymer (Guildford) 52 (2011): 4656–4663.
<https://dx.doi.org/10.1016/j.polymer.2011.08.045>

51)-Biotic and inorganic control on travertine deposition at Bullicame 3 spring (Viterbo, Italy): A multidisciplinary approach

Di Benedetto F; Montegrossi G; Minissale A; Pardi L; Romanelli M; Tassi F; Huertas AD; Pampin EM; Vaselli O; Borrini D
Geochimica et cosmochimica acta 75 (2011): 4441–4455.
<https://dx.doi.org/10.1016/j.gca.2011.05.011>

52)-Corrigendum to: "Investigation of alkyl metal intermediates formation in the rhodium-catalyzed hydro-formylation: experimental and theoretical approaches" [Coord. Chem. Rev. 254 (2010) 696-706]

Raffaello Lazzaroni; Roberta Settambolo; Giuliano Alagona; Caterina Ghio

Coordination chemistry reviews (Print) 255 (2011): 3031–3031.

<https://dx.doi.org/10.1016/j.ccr.2011.06.008>

53)-THz-Waves Channeling in a Monolithic Saddle-Coil for Dynamic Nuclear Polarization enhanced NMR

Macor, A; de Rijk, E; Annino, G; Alberti, S; Ansermet, J-Ph

Journal of magnetic resonance (S.-Diego, Calif., 1997 : Online) 212 (2011): 440–449.

<http://www.cnr.it/prodotto/i/197541>

info:cnr-pdr/source/autori:Macor, A; de Rijk, E; Annino, G; Alberti, S; Ansermet, J-Ph/titolo:THz-Waves Channeling in a Monolithic Saddle-Coil for Dynamic Nuclear Polarization enhanced NMR/

54)-Virtual Experiments by Pulse Heating Techniques: Cylindrical Tungsten Specimens

Bussolino, GC; Annino, G; Ferrari, C; Righini, F

International journal of thermophysics (Dordr., Online) 32 (2011): 2716–2726.

<http://www.cnr.it/prodotto/i/197544>

info:cnr-pdr/source/autori:Bussolino, GC; Annino, G; Ferrari, C; Righini, F/titolo:Virtual Experiments by Pulse Heating Techniques: Cylindrical Tungsten Specimens/

55)-Tocopherol speciation as first screening for the assessment of extra virgin olive oil quality by reversed-phase high-performance liquid chromatography/fluorescence detector

Chen Huilun [1,2,3]; Angiuli Marco [4]; Ferrari Carlo [5]; Tombari Elpidio [4]; Salvetti Giuseppe [4]; Bramanti Emilia [1]subjectAuthenticationsubjectAdulterationsubjectExtra virgin olive oilsubjectHPLCsubjectTocopherols

Food chemistry 125 (2011): 1423–1429.

<https://dx.doi.org/10.1016/j.foodchem.2010.10.026>

56)-Effect of polymerization on the boson peak, from liquid to glass

S. Caponi (a,b); S. Corezzi (c,d); D. Fioretto (c); A. Fontana (a,e); G. Monaco (f); F. Rossi (a,e)subjectGlass transitionssubjectPolymerizationsubjectRaman ScatteringsubjectVibrational density of state

Journal of non-crystalline solids 357 (2011): 530–533.

<https://dx.doi.org/10.1016/j.jnoncrysol.2010.06.069>

57)-Effect of elastic properties modification on the vibrational density of states: A joint Brillouin and Raman scattering study

S. Caponi; S. Corezzi; D. Fioretto; A. Fontana; F. Rossisubjectdegree of polymerization (DP)subjectglass transitionsubjectRaman spectroscopysubjectresinssubjectviscoelastic properties

Journal of applied polymer science (Print) 122 (2011): 3672–3676.

<https://dx.doi.org/10.1002/app.34780>

58)-Unravelling the detailed microstructure of a semiconducting (quasi-metal) soluble polymer incorporating conjugated thienylene methine sequences

P. Stagnaro; M. Panizza; A. Gandini; D. Prevosto; M. Lucchesi

Journal of polymer science. Part A, Polymer chemistry 49 (2011): 5227–5238.

<https://dx.doi.org/10.1002/pola.24993>

59)-Effect of Confinement on Structural Relaxation in Ultrathin Polymer Films Investigated by Local Dielectric Spectroscopy

Nguyen, Hung K.; Prevosto, Daniele; Labardi, Massimiliano; Capaccioli, Simone; Lucchesi, Mauro; Rolla, Pierangelo

Macromolecules (Print) 44 (2011): 6588–6593.

<https://dx.doi.org/10.1021/ma200440z>

60)-Ab initio study of excited state electronic circular dichroism. Two prototype cases: Methyl oxirane and R-(+)-1,1'-bi(2-naphthol)

Rizzo, Antonio; Vahtras, Olav
subjectab initio calculations
subjectcircular dichroism
subjectdensity functional theory
subjectelectron correlations
subjectexcited states
subjectHF calculations
subjectmolecular configuration
subjectmolecular electronic states
subjectmolecule-photon collisions
subjectoptical rotations
subjectorganic compound
subjectphotoexcitations
subjectSCF calculations
subjecttime resolved spectra

The Journal of chemical physics 134 (2011): 244109.

<https://dx.doi.org/10.1063/1.3602219>

61)-Elastic anomalies at terahertz frequencies and excess density of vibrational states in silica glass

Baldi, Giacomo; Giordano, Valentina M.; Monaco, Giulio

Physical review. B, Condensed matter and materials physics 83 (2011): 174203.

<https://dx.doi.org/10.1103/PhysRevB.83.174203>

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Other publications (journals without peer review, book reviews,etc.)

1)-Excess Enthalpies of Mixtures of Linear Monocarboxylic Acids with Dibutylether. Comparison with DISQUAC Predictions.

Falconieri D.; Marongiu B.; Piras A.; Porcedda S.; Lepori L.; Matteoli E.

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info:cnr-pdr/source/autori:Falconieri D., Marongiu B., Piras A., Porcedda S., Lepori L. and Matteoli E./congresso_nome:Proceedings of Medicta 2011 (10th mediterranean Conference on Calorimetry and Thermal Analysis)/congresso_luogo:Porto/congresso_data:2011/anno:2011/pagina_da:/pagina_a:/intervallo_pagine:

2)-Thermodynamics of Complex Formation Reactions of 18-Crown-6 Ether with Some Amino Acids in Water-Dimethylsulfoxide Mixtures

Chernov I.V.; Usacheva T.R.; Kuzmina I.A.; Sharnin V.A.; Matteoli E.

XIX Congress on General & Applied Chemistry, Volgograd, 2011

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3)-Efforts to understand the mechanical behaviour of composite materials from biodegradable polyesters and hemp fibres as a consequence of the structural and chemical features of the fibres

S. Bronco; F. Signori; M. Pelagaggi; F. Ciardelli

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4)-Particle Kinetics in Asymmetric Solitary Waves

NOCERA L; PALUMBO L JsubjectSolitary wavessubjectdouble layerssubjectBGK wavessubjectsheathsubjectasymmetry

pp.1-9, 2011

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5)-Composites from biodegradable polyesters and hemp fibers: an effort towards the enlightenment of polymer matrix-fiber interactions

Signori F.; Pelagaggi M.; Righetti M.C.; Bronco S.; Ciardelli F.

Hybrid Materials 2011, Strasbourg (France), 2011

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6)-New Functional Materials from Polysaccharides Modified by Copper Catalyzed Azide-Alkyne Cycloaddition

M. Bertoldo; G. Zampano; S. Nazzi; F. La Terra; F. Ciardelli

European Polymer Congress 2011 (EPF2011) & XII Congress of the Specialized Group of Polymers (XII GEP Congress), Granada-Spain, June 26 - July 1

<http://www.cnr.it/prodotto/i/192633>

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7)-Hyperpolarization and Multiple Irradiation Probe Head for Magnetic Resonance Techniques

Annino, G;

PCT/EP2011/060856, PCT/EP2012/062492, Internazionale

<http://www.cnr.it/prodotto/i/197643>

8)-Over-moded resonant cavities for low dissipative magnetic resonance probes based on photonic band structures

Macor, A;

PCT/IB2011/054620, PCT/IB2012/055694, Internazionale

<http://www.cnr.it/prodotto/i/197648>

9)-Caratterizzazione della SLC: Proprieta e alterazioni chimico-fisiche

Romanelli, M. (1); Bartali, L.(1); Di Benedetto, F.(1); Innocenti, M.(1); Tesi, S.(1); Bafaro, E.(2); Fornaciai, G.(2); D'Acapito, F. (3); Montegrossi, G.(4); Pardi, L.A. (5)subjectSilica pollutionsubjectfree silicasubjectchemical propertiessubjectphysical properties

Silice libera cristallina nei luoghi di lavoro. I contributi dei progetti finalizzati della Regione Toscana (2004-2009) nel campo della prevenzione, dell'igene industriale, della ricerca e dell'epidemiologia, edited by Capacci F.; Carnevale F.; Di Benedetto F., pp. 192–275, 2011

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10)-NONLINEAR CHIROPTICAL PROPERTIES AND SPECTROSCOPIES

Antonio Rizzo

7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda University, Tokyo, Japan, 2-8 Settembre, 2011

<http://www.cnr.it/prodotto/i/300369>

info:cnr-pdr/source/autori:Antonio Rizzo/congresso_nome:7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII)/congresso_luogo:Waseda University, Tokyo, Japan/congresso_data:2-8 Settembre, 2011/anno:2011/pagina_da:/pagina_a:/intervallo_pagine:

11)-NONLINEAR SPECTROSCOPIES AND CHIRALITY

Antonio Rizzo

47th Symposium on Theoretical Chemistry (STC 2011). Designing Molecular Functionality: Challenges for Theoretical Approaches, Sursee, Switzerland, 21-25 Agosto 2011

<http://www.cnr.it/prodotto/i/300372>

info:cnr-pdr/source/autori:Antonio Rizzo/congresso_nome:47th Symposium on Theoretical Chemistry (STC 2011). Designing Molecular Functionality: Challenges for Theoretical Approaches/congresso_luogo:Sursee, Switzerland/congresso_data:21-25 Agosto 2011/anno:2011/pagina_da:/pagina_a:/intervallo_pagine:

12)-NONLINEAR SPECTROSCOPIES AND CHIRALITY

Antonio Rizzo

Ninth Triennial Congress of The World Association of Theoretical and Computational Chemists - WATOC 2011, University of Santiago de Compostela, Santiago de Compostela, Spain, 17-22 Luglio, 2011

<http://www.cnr.it/prodotto/i/300375>

info:cnr-pdr/source/autori:Antonio Rizzo/congresso_nome:Ninth Triennial Congress of The World Association of Theoretical and Computational Chemists - WATOC 2011/congresso_luogo:University of Santiago de Compostela, Santiago de Compostela, Spain/congresso_data:17-22 Luglio, 2011/anno:2011/pagina_da:/pagina_a:/intervallo_pagine:

13)-NON-LINEAR SPECTROSCOPIES AND CHIRALITY

Antonio Rizzo

"Holistic Computational Spectroscopy: innovative concepts, modern tools, strategic vision and challenges" -CODECS Workshop, Scuola Normale Superiore, Pisa, Italia, 16-18 Novembre 2011

<http://www.cnr.it/prodotto/i/300387>

info:cnr-pdr/source/autori:Antonio Rizzo/congresso_nome:"Holistic Computational Spectroscopy: innovative concepts, modern tools, strategic vision and challenges" -CODECS Workshop/congresso_luogo:Scuola Normale Superiore, Pisa, Italia/congresso_data:16-18 Novembre 2011/anno:2011/pagina_da:/pagina_a:/intervallo_pagine:

14)-Particle Kinetics in Asymmetric Electrostatic Waves

Nocera L; Palumbo LJsubjectSolitary wavessubjectdouble layerssubjectBGK wavessubjectsheathssubjectasymmetrysubjectdistribution functionssubjectdiscontinuitysubjectlogarithmic singularitysubjectVlasov equation pp.1-18, 2011

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