

## Peer-reviewed journal articles

### 1)-Coherent effects on the Zeeman sublevels of hyperfine states at the D1 and D2 lines of Rb

Alzetta G. 1; Cartaleva S. 2; Dancheva Y. 2; Andreeva Ch. 2; Gozzini S. 3; Botti L. 1 Rossi A. 1  
SUBJECTAtomic coherenceSUBJECTcoherent populationSUBJECTOptical pumping  
*Journal of optics. B, Quantum and semiclassical optics (Print)* 3 (2001): 181–188.  
<https://dx.doi.org/10.1088/1464-4266/3/3/317>

### 2)-Evaluating the magnetic anisotropy in molecular rare earth compounds. Gadolinium derivatives with semiquinone radical and diamagnetic analogues

Caneschi A.; Dei A.; Gatteschi D.; Massa C.A.; 1; Pardi L.A.; 1; Poussereau S.; Sorace L.  
SUBJECTEPRSUBJECTMagneticSUBJECTSpinSUBJECTLanthanidesSUBJECTSemiquinones  
*Chemical physics letters (Print)* 371 (2001): 694–699.  
<http://www.cnr.it/prodotto/i/39206>

info:cnr-pdr/source/autori:Caneschi A., Dei A., Gatteschi D., Massa C.A., 1, Pardi L.A., 1, Poussereau S., Sorace L./titolo:Evaluating the magnetic anisotropy in molecular rare earth compounds. Gadolinium derivatives with semiquinone radical and diamagnetic analogues/

### 3)-The combined effects of temperature and polymerization rate changes on the real-time conduction and relaxation of a liquid, and the evolution of localized motions

Cardelli C. (1); Tombari E. (1); Johari G.P. (2)  
SUBJECTDIELECTRIC-RELAXATIONSUBJECTMOLECULAR-DYNAMICSSUBJECTCALORIMETRYSUBJECTMACROMOLECULES GROWTHSUBJECTTHERMOSET  
*105 (2001): 11035–11043.*  
<http://www.cnr.it/prodotto/i/39210>

info:cnr-pdr/source/autori:Cardelli C. (1), Tombari E. (1), Johari G.P. (2)/titolo:The combined effects of temperature and polymerization rate changes on the real-time conduction and relaxation of a liquid, and the evolution of localized motions/

### 4)-Controlled dumping of pulses of laser radiation ranging from MIR to the FIR by means of optical semiconductor switching

Marchetti S.; Martinelli M.; Simili R.; Giorgi M.; Fantoni R.  
SUBJECTinfrarossoSUBJECTimpulsi cortiSUBJECTalta potenza  
*72 (2001): 927–930.*  
<http://www.cnr.it/prodotto/i/39262>

info:cnr-pdr/source/autori:Marchetti S., Martinelli M., Simili R., Giorgi M., Fantoni R./titolo:Controlled dumping of pulses of laser radiation ranging from MIR to the FIR by means of optical semiconductor switching/

**5)-The effect of time-dependent random mass density field on frequencies of solar sound waves**

MURAWSKI K; NOCERA L; MEDREK MSUBJECTSun: convectionSUBJECTturbulenceSUBJECTglobal oscillationsSUBJECTrandom media  
*Astronomy & astrophysics (Print)* 376 (2001): 708–712.  
<https://dx.doi.org/10.1051/0004-6361:20011030>

**6)-Solar acoustic oscillations in a random density field**

NOCERA L; MEDREK M; MURAWSKI KSUBJECTsolar global oscillationsSUBJECTturbulent mediaSUBJECTturbulent mediaSUBJECTLandau damping  
*Astronomy & astrophysics (Print)* 373 (2001): 301–306.  
<https://dx.doi.org/10.1051/0004-6361:20010513>

**7)-Ab Initio Modelling of Competitive Drug-Drug Interactions: 5-Fluorouracil Dimers in the Gas Phase and in Solution.**

Alagona\* G.; Ghio C.; Monti S.SUBJECTH-bond interactionsSUBJECTstacking interactionsSUBJECTcorrelation correctionsSUBJECTBSSE, thermal correctionsSUBJECTcontinuum solvent effect  
*International journal of quantum chemistry* 83 (2001): 128–142.  
<http://www.cnr.it/prodotto/i/39680>

info:cnr-pdr/source/autori:Alagona\* G., Ghio C., Monti S./titolo:Ab Initio Modelling of Competitive Drug-Drug Interactions: 5-Fluorouracil Dimers in the Gas Phase and in Solution./

**8)-Reaction mechanisms between methylamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO)**

Alagona\* G.; Ghio C.SUBJECTpyridoxalphosphateSUBJECTtopaquinoneSUBJECTbenzylamine Schiff basesSUBJECTtransamination reactionSUBJECTaminotransferase mechanism  
*International journal of quantum chemistry* 84 (2001): 740–749.  
<http://www.cnr.it/prodotto/i/39681>

info:cnr-pdr/source/autori:Alagona\* G., Ghio C./titolo:Reaction mechanisms between methylamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO)/

**9)-Olefin Insertion into the Rhodium-Hydrogen Bond as the Step Determining the Regioselectivity of Rhodium-Catalyzed Hydroformylation of Vinyl Substrates: Comparison between Theoretical and Experimental Results**

Alagona\* G.; Ghio C.; Lazzaroni R.; Settambolo R.SUBJECTRegioselectivitySUBJECTComputational predictionSUBJECThydroformylationSUBJECTunmodified rhodium catalystsSUBJECTreaction mechanism  
*Organometallics* 20 (2001): 5394–5404.  
<http://www.cnr.it/prodotto/i/39682>

info:cnr-pdr/source/autori:Alagona\* G., Ghio C., Lazzaroni R., Settambolo R./titolo:Olefin Insertion into the Rhodium-Hydrogen Bond as the Step Determining the Regioselectivity of Rhodium-Catalyzed Hydroformylation of Vinyl Substrates: Comparison between Theoretical and Experimental Results/

**10)-A screened static-exchange potential for core electron excitations**

V. Carravetta; O. Plashkevych; Hans AgrenSUBJECTtheorySUBJECTcomputational chemistrySUBJECTcore excitationSUBJECTNEXAFSSUBJECTXAS

*Chemical physics (Print) 263 (2001): 231–242.*

<http://www.cnr.it/prodotto/i/39940>

info:cnr-pdr/source/autori:V. Carravetta, O. Plashkevych and Hans Agren/titolo:A screened static-exchange potential for core electron excitations/

**11)-Gas-phase experimental and theoretical near edge X-ray absorption fine structure study of 2-mercaptobenzothiazole**

G. Contini; V. Carravetta; V. Di-Castro; S. Stranges; R. Richter; M. AlagiaSUBJECTtheorySUBJECTexperimentSUBJECTNEXAFSSUBJECTXASSUBJECT2-mercaptobenzothiazole

*The journal of physical chemistry. A 105 (2001): 7308–7314.*

<https://dx.doi.org/10.1021/jp010865e>

**12)-Dynamical suppression of atomic peaks in resonant dissociative photoemission**

P. Salek; V. Carravetta; FK Gel'mukhanov; H. Agren; B. Schimmelpfennig; MN Piancastelli L. Sorensen; R. Feifel; I. Hjelte; M. Bassler; S. Svensson; O. Bjorneholm; A. de-BritoSUBJECTtheorySUBJECTresonant Auger

decaySUBJECTHFSUBJECTdissociationSUBJECTatomic peaks

*Chemical physics letters (Print) 343 (2001): 332–338.*

<http://www.cnr.it/prodotto/i/39942>

info:cnr-pdr/source/autori:P. Salek, V. Carravetta, FK Gel'mukhanov, H. Agren, B. Schimmelpfennig, MN Piancastelli L. Sorensen, R. Feifel, I. Hjelte, M. Bassler, S. Svensson, O. Bjorneholm, A. de-Brito/titolo:Dynamical suppression of atomic peaks in resonant dissociative photoemission/

**13)-Photoelectron spectroscopy (PES) study of gas-phase 2,5-(2,2'-dithienyl)diethynylthiophene (TRIM): an experimental and theoretical study**

G. Polzonetti; V. Carravetta; A. Ferri; P. Altamura; M. Alagia; R. Richter; M.V. RussoSUBJECTexperimentSUBJECTtheorySUBJECTXPSSUBJECT2,5-(2,2'-dithienyl)diethynyl-thiophene

*Chemical physics letters (Print) 340 (2001): 449–457.*

<http://www.cnr.it/prodotto/i/39943>

info:cnr-pdr/source/autori:G. Polzonetti, V. Carravetta, A. Ferri, P. Altamura, M. Alagia, R. Richter, and M.V. Russo/titolo:Photoelectron spectroscopy (PES) study of gas-phase 2,5-(2,2'-dithienyl)diethynyl-thiophene (TRIM): an experimental and theoretical study/

**14)-The Cotton-Mouton effect of gaseous CO<sub>2</sub>, N<sub>2</sub>O, OCS and CS<sub>2</sub>. A Cubic Response MCSCF study**

Jonsson, D.; Norman, P.; Ågren, H.; Rizzo, A.; Coriani, S.; Ruud, K.

*114 (2001): 8372–8381.*

<http://www.cnr.it/prodotto/i/40328>

info:cnr-pdr/source/autori:Jonsson, D.; Norman, P.; Ågren, H.; Rizzo, A.; Coriani, S.; Ruud, K./titolo:The Cotton-Mouton effect of gaseous CO<sub>2</sub>, N<sub>2</sub>O, OCS and CS<sub>2</sub>. A Cubic Response MCSCF study/

**15)-Coupled Cluster calculation of dispersion contributions to interaction energies and polarizabilities.**

Jaszunski, M.; Rizzo, A.; Jørgensen, P.

*116 (2001): 251–258.*

<http://www.cnr.it/prodotto/i/40329>

info:cnr-pdr/source/autori:Jaszunski, M.; Rizzo, A.; Jørgensen, P./titolo:Coupled Cluster calculation of dispersion contributions to interaction energies and polarizabilities./

**16)-The Cotton-Mouton effect of gaseous N<sub>2</sub>, CO, CO<sub>2</sub>, N<sub>2</sub>O, OCS and CS<sub>2</sub>: a density functional approach to high-order mixed electric and magnetic properties**

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

*Chemical physics letters (Print) 346 (2001): 251–258.*

<http://www.cnr.it/prodotto/i/40330>

info:cnr-pdr/source/autori:Cappelli, C.; Mennucci, B.; Tomasi, J.; Cammi, R.; Rizzo, A./titolo:The Cotton-Mouton effect of gaseous N<sub>2</sub>, CO, CO<sub>2</sub>, N<sub>2</sub>O, OCS and CS<sub>2</sub>: a density functional approach to high-order mixed electric and magnetic properties/

**17)-Volumetric properties of (an organic compound + di-n-butyl ether) at 298.15K**

Bernazzani L.; Ceccanti N.; Conti. G; Gianni P.; Mollica V.; Tinè M.R.; Lepori L.; Matteoli E.; Spanedda A.

*Journal of Chemical Thermodynamics 33 (2001): 629–641.*

<http://www.cnr.it/prodotto/i/40528>

info:cnr-pdr/source/autori:Bernazzani L., Ceccanti N., Conti. G, Gianni P., Mollica V., Tinè M.R., Lepori L., Matteoli E., Spanedda A./titolo:Volumetric properties of (an organic compound + di-n-butyl ether) at 298.15K/

**18)-Dielectric relaxation and the conformer equilibrium in the liquid and glassy states of b-D-fructose**

Tombari E.; Cardelli C.; Salvetti G.; Johari G.P.

*Journal of molecular structure (Print) 559 (2001): 245–254.*

<http://www.cnr.it/prodotto/i/40603>

info:cnr-pdr/source/autori:Tombari E., Cardelli C., Salvetti G., Johari G.P./titolo:Dielectric relaxation and the conformer equilibrium in the liquid and glassy states of b-D-fructose/

**19)-Free space excitation of novel “fractional” whispering gallery mode dielectric resonators**

Annino G.; Cassettari M.; Martinelli M.

*Applied magnetic resonance* (2001).

<http://www.cnr.it/prodotto/i/40651>

info:cnr-pdr/source/autori:Annino G., Cassettari M., Martinelli M./titolo:Free space excitation of novel “fractional” whispering gallery mode dielectric resonators/

**20)-Complex response function of whispering gallery dielectric resonators**

Annino G.; Cassettari M.; Fittipaldi M.; Martinelli M.

*International journal of infrared and millimeter waves* (2001).

<http://www.cnr.it/prodotto/i/40652>

info:cnr-pdr/source/autori:Annino G., Cassettari M., Fittipaldi M., Martinelli M./titolo:Complex response function of whispering gallery dielectric resonators/

**21)-The electric-field-gradient-induced birefringence and the determination of molecular quadrupole moments**

Coriani, S.; Halkier, A.; Rizzo, A.

*J Chem Phys* (2001): 1–21.

<http://www.cnr.it/prodotto/i/66441>

info:cnr-pdr/source/autori:Coriani, S.; Halkier, A.; Rizzo, A./titolo:The electric-field-gradient-induced birefringence and the determination of molecular quadrupole moments/

**22)-Synchrotron radiation photoemission study of some p-conjugated alkynes in the gas phase: Experiment and theory**

V. Carravetta; G. Iucci; A. Ferri; M.V. Russo; S. Stranges; M. de Simone; G. Polzonetti

*Chemical physics (Print)* 264 (2001): 175–186.

[https://dx.doi.org/10.1016/S0301-0104\(00\)00396-7](https://dx.doi.org/10.1016/S0301-0104(00)00396-7)

**23)-Enantioselective alternating terpolymerization of propene and ethene with carbon monoxide**

Sesto, B; Bronco, S; Gindro, EL; Consiglio, G

*Macromolecular chemistry and physics (Print)* 20 (2001): 2059–2064.

[https://dx.doi.org/10.1002/1521-3935\(20010601\)202:10<2059::AID-MACP2059>3.0.CO;2-K](https://dx.doi.org/10.1002/1521-3935(20010601)202:10<2059::AID-MACP2059>3.0.CO;2-K)

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

**1)-Drug Delivery by Biodegradable Poly(Ester-Ether-Ester)s: a Tentative Theoretical Evaluation of the Interactions between Drug and Macromolecular Matrix**

Alagona G.(1); Ghio C.(1); Monti S.(1); Guerra G.D.(2); Maltinti S.(3)  
, 2001

<http://www.cnr.it/prodotto/i/137248>

info:cnr-pdr/source/autori:Alagona G.(1), Ghio C.(1), Monti S.(1), Guerra G.D.(2), Maltinti S.(3)/titolo:Drug Delivery by Biodegradable Poly(Ester-Ether-Ester)s: a Tentative Theoretical Evaluation of the Interactions between Drug and Macromolecular Matrix/titolo\_volume:/curatori\_volume:/editore:/anno:2001

**2)-Atoms, Molecules and Quantum Dots in Laser Fields: Fundamental Processes**

Bloembergen, N.; Rahman, N.; Rizzo, A.

2001

<http://www.cnr.it/prodotto/i/137284>

info:cnr-pdr/source/autori:Bloembergen, N.; Rahman, N.; Rizzo, A./titolo:Atoms, Molecules and Quantum Dots in Laser Fields: Fundamental Processes/editore:/anno:2001