Peer-reviewed journal articles

1)-Risk Assessment and Risk Minimization in Nanomedicine: A Need for Predictive, Alternative, and 3Rs Strategies

Accomasso, Lisa; Cristallini, Caterina; Giachino, Claudiasubjectnanomaterialsubjectnanomedicinesubjectnanosafetysubjectrisk assessmentsubjectrisk minimization

Frontiers in Pharmacology 9 (2018).

https://dx.doi.org/10.3389/fphar.2018.00228

2)-Predicting the helical sense of Poly(phenylacetylene)s from their Electron Circular Dichroism Spectra

B. Fernández; R. Rodríguez; A. Rizzo; E. Quiñoá; R. Riguera; F. FreiresubjectDicroismo Circolare ElettronicosubjectPolifenilacetilenisubjectTD-DFT

Angewandte Chemie (Int. ed., Print) 57 (2018): 3666–3670.

https://dx.doi.org/10.1002/anie.201713164

3)-Predicting the Helical Sense of Poly(phenylacetylene)s from their Electron Circular Dichroism Spectra

B. Fernández; R. Rodríguez; A. Rizzo; E. Quiñoá; R. Riguera; F. FreiresubjectDicroismo Circolare ElettronicosubjectPolienilacetilenisubjectTD-DFT

Angewandte Chemie (Print) 130 (2018): 3728–3732.

https://dx.doi.org/10.1002/ange.201713164

4)-A QM/MM and QM/QM/MM study of Kerr, Cotton-Mouton and Jones linear birefringences in liquid acetonitrile

T. Fahleson; J. M. H. Olsen; P. Norman; A. RizzosubjectQM/MMsubjectPolarizable Density EmbeddingsubjectLinear BirefringencessubjectJones BirefringencesubjectAcetonitrile

PCCP. Physical chemistry chemical physics (Print) 20 (2018): 3831–3840.

https://dx.doi.org/10.1039/C7CP07421B

5)-Quantum Effects for a Proton in a Low-Barrier, Double-Well Potential: Core Level Photoemission Spectroscopy of Acetylacetone

Feyer, Vitaliy; Feyer, Vitaliy; Prince, Kevin C.; Prince, Kevin C.; Coreno, Marcello; Melandri, Sonia; Maris, Assimo; Evangelisti, Luca; Caminati, Walther; Giuliano, Barbara M.; Giuliano, Barbara M.; Kjaergaard, Henrik G.; Carravetta, Vincenzosubjectcore photoemission spectroscopysubjectcomputational spectroscopysubjectacetylacetonesubjectintramolecular hydrogen bond

The journal of physical chemistry letters 9 (2018): 521–526.

https://dx.doi.org/10.1021/acs.jpclett.7b03175

6)-**Molecular dynamics simulations of melting and sintering of Si nanoparticles: A comparison of different force fields and computational models**

Sementa L.; Barcaro G.; Monti S.; Carravetta V.subjectsilicon nanoparticles; molecular dynamics

PCCP. Physical chemistry chemical physics (Print) 20 (2018): 1707–1715.

https://dx.doi.org/10.1039/c7cp07583a

7)-**Fluorescent LDPE and PLA nanocomposites containing fluorescein-modified layered double hydroxides and their ON/OFF responsive behavior towards humidity**

Coiai, Serena; Javarone, Stefano; Cicogna, Francesca; Oberhauser, Werner; Onor, Massimo; Pucci, Andrea; Minei, Pierpaolo; Iasilli, Giuseppe; Passaglia, ElisasubjectFluorescein co-intercalated layered double hydroxidessubjectFluorescent polymer-based nanocompositessubjectOptical propertiessubjectResponsiveness to humidity

European Polymer Journal 99 (2018): 189–201.

https://dx.doi.org/10.1016/j.eurpolymj.2017.12.021

8)-**Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: Au<inf>36-x</inf>Ag<inf>x</inf>(SPh-tBu)<inf>24</inf>**

Theivendran, Shevanuja; Chang, Le; Mukherjee, Aneek; Sementa, Luca; Stener, Mauro; Fortunelli, Alessandro; Dass, AmalasubjectDENSITY-FUNCTIONAL THEORYsubjectCHIROPTICAL PROPERTIESsubjectGOLD-SILVER NANOPARTICLESsubjectTHEORETICAL-ANALYSISsubjectNANOALLOYS

Journal of physical chemistry. C 122 (2018): 4524–4531.

https://dx.doi.org/10.1021/acs.jpcc.8b00556

9)-**Ligand Structure Determines Nanoparticles' Atomic Structure, Metal-Ligand Interface and Properties**

Rambukwella, Milan; Sakthivel, Naga Arjun; Delcamp, Jared H.; Sementa, Luca; Fortunelli, Alessandro; Dass, Amalasubjectligand effectsubjectnanoparticle atomic structuresubjectmetal ligand interfacesubjectligand-ligand interactionsubjectnanoparticle synthesis

Frontiers in Chemistry 6 (2018): 1–17.

https://dx.doi.org/10.3389/fchem.2018.00330

10)-**Individual Component Map of Rotatory Strength and Rotatory Strength Density Plots As Analysis Tools of Circular Dichroism Spectra of Complex Systems**

Chang, Le; Baseggio, Oscar; Sementa, Luca; Cheng, Daojian; Fronzoni, Giovanna; Toffoli, Daniele; Aprà, Edoardo; Stener, Mauro; Fortunelli, Alessandrosubjecttime-dependent density functional theorysubjectmonolayer-protected clusters

Journal of chemical theory and computation 14 (2018): 3703–3714.

https://dx.doi.org/10.1021/acs.jctc.8b00250

11)-Time-dependent density-functional study of the photoabsorption spectrum of Au<inf>25</inf>(SC<inf>2</inf>H<inf>4</inf>C<inf>6</inf>H<inf>5</inf>)<inf>18</inf>anion: Validation of the computational protocol

Baseggio, Oscar; De Vetta, Martina; Fronzoni, Giovanna; Toffoli, Daniele; Stener, Mauro; Sementa, Luca; Fortunelli, Alessandrosubjectmonolayer-protected clusterssubjecttime-dependent density functional theory

International journal of quantum chemistry 118 (2018): 1–9.

https://dx.doi.org/10.1002/qua.25769

12)-Evidence of a low-temperature dynamical transition in concentrated microgels

Zanatta M.; Tavagnacco L.; Buratti E.; Bertoldo M.; Natali F.; Chiessi E.; Orecchini A.; Zaccarelli E.subjectAcrylic monomerssubjectAmidessubjectIncoherent scatteringsubjectMolecular dynamicssubjectNeutron scatteringsubjectProteins

Science Advances 4 (2018).

https://dx.doi.org/10.1126/sciadv.aat5895

13)-Interpenetrating Polymer Network Microgels in Water: Effect of Composition on the Structural Properties and Electrosteric Interactions

Micali N.; Bertoldo M.; Buratti E.; Nigro V.; Angelini R.; Villari V.subjectcolloidal propertiessubjectelectrosteric interactionssubjectmicrogelsubjectNMR spectroscopysubjectpolymer network

ChemPhysChem (Print) 19 (2018): 2894–2901.

https://dx.doi.org/10.1002/cphc.201800707

14)-TDDFT Study of the Optical Spectra of Free and Supported Binary Coinage Metal Hexamers: Effect of Doping and Support

Luque-Ceballos J.C.; Sementa L.; Apra E.; Fortunelli A.; Posada-Amarillas A.subjecttime-dependent density-functional theorysubjectclusters

Journal of physical chemistry. C 122 (2018): 23143–23152.

https://dx.doi.org/10.1021/acs.jpcc.8b06397

15)-Structure and Dynamics of Biobased Polyester Nanocomposites

Krystalenia Androulaki; Kiriaki Chrissopoulou; Daniele Prevosto; Massimiliano Labardi; Spiros H. Anastasiadissubjectpolyestersubjectnanocompositesubjectsilicatesubjectdielectric spectroscopysubjectpolyol

Biomacromolecules (Online) (2018).

https://dx.doi.org/10.1021/acs.biomac.8b01231

16)-TiO2-SiO2-PDMS nanocomposite coating with self-cleaning effect for stone material: Finding the optimal amount of TiO2

Crupi, Vincenza; Fazio, Barbara; Gessini, Alessandro; Kis, Zoltan; La Russa, Mauro F.; Majolino, Domenico; Masciovecchio, Claudio; Ricca, Michela; Rossi, Barbara; Ruffolo, Silvestro A.; Venuti, ValentinasubjectTitanium dioxidesubjectNanostructured

coatingssubjectPhotocatalyticssubjectNeutron radiographysubjectSR-RamansubjectCultural heritage
Construction & building materials 166 (2018): 464–471.
https://dx.doi.org/10.1016/j.conbuildmat.2018.01.172

17)-Crystallization-induced formation of rigid amorphous fraction
Maria Laura Di Lorenzo; Maria Cristina Righettisubjectcalorimetrysubjectpolymer crystallizationsubjectrigid amorphous fraction
Polymer crystallization Online 1 (2018).
https://dx.doi.org/10.1002/pcr2.10023

18)-Au<inf>279</inf>(SR)<inf>84</inf>: The Smallest Gold Thiolate Nanocrystal That Is Metallic and the Birth of Plasmon
Sakthivel, Naga Arjun; Stener, Mauro; Sementa, Luca; Fortunelli Alessandro; Ramakrishna, Guda; Dass, AmalasubjectOPTICAL PROPERTIESsubjectCRYSTAL STRUCTUREsubjectQUANTUM CONFINEMENTsubjectGOLD NANOPARTICLESsubjectNANOCLUSTERSsubjectNANOMOLECULESsubjectELECTRON DYNAMICS
The journal of physical chemistry letters 9 (2018): 1295–1300.
https://dx.doi.org/10.1021/acs.jpclett.8b00308

19)-Bimetallic Ag-Pt sub-nanometer supported clusters as highly efficient and robust oxidation catalysts
Negreiros, Fabio R.; Halder, Avik; Yin, Chunrong; Singh, Akansha; Barcaro, Giovanni; Sementa, Luca; Tyo, Eric C.; Pellin, Michael J.; Bartling, Stephan; Meiwes-Broer, Karl-Heinz; Seifert, Sönke; Sen, Prasenjit; Nigam, Sandeep; Majumder, Chiranjib; Fukui, Nobuyuki; Yasumatsu, Hisato; Vajda, Stefan; Fortunelli Alessandrosubjectsubnanometer catalystssubjectoxidation catalysissubjectreactive glocal optimization
Angewandte Chemie (Int. ed., Print) 57 (2018): 1209–1213.
https://dx.doi.org/10.1002/anie.201709784

20)-Bimetallic Ag-Pt sub-nanometer supported clusters as highly efficient and robust oxidation catalysts
Negreiros, Fabio R.; Halder, Avik; Yin, Chunrong; Singh, Akansha; Barcaro, Giovanni; Sementa, Luca; Tyo, Eric C.; Pellin, Michael J.; Bartling, Stephan; Meiwes-Broer, Karl-Heinz; Seifert, Sönke; Sen, Prasenjit; Nigam, Sandeep; Majumder, Chiranjib; Fukui, Nobuyuki; Yasumatsu, Hisato; Vajda, Stefan; Fortunelli Alessandrosubjectultrananocatalystssubjectreactive glocal optimization
Angewandte Chemie (Print) 130 (2018): 1223–1227.
https://dx.doi.org/10.1002/ange.201709784

21)-Hydrogen evolution reaction (HER) on Au@Ag ultrananoclusters as electro-catalysts

Chang L.; Cheng D.; Sementa L.; Fortunelli AlessandrosubjectHER reaction; calculations; Ag-Au subnanometer clusters
Nanoscale (Print) 10 (2018): 17730–17737.
https://dx.doi.org/10.1039/c8nr06105j

22)-SERS amplification by ultra-dense plasmonic arrays on self-organized PDMS templates
Repetto, Diego; Giordano, Maria Caterina; Foti, Antonino; Gucciardi, Pietro Giuseppe; Mennucci, Carlo; de Mongeot, Francesco BuatiersubjectPolydimethylsiloxane (PDMS)subjectSoft lithographysubjectPlasmonic nanostructuresubjectSurface-enhanced Raman spectroscopy (SERS)subjectOptical dichroism
Applied surface science 446 (2018): 83–91.
https://dx.doi.org/10.1016/j.apsusc.2018.02.163

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

1)-Electrostatic Force Microscopy Techniques for Interphase Characterization

Massimiliano Labardi; Daniele Prevosto; Simone Capacciolisubjectelectrostatic force microscopy; atomic force microscopy; interfaces; nanocomposites; hybrid materials

Hybrid Organic-Inorganic Interfaces: Towards Advanced Functional Materials, edited by Delville Marie Helene, Taubert Andreas, pp. 867. New York: J. Wiley & sons, 2018

urn:isbn:978-3-527-34255-6

info:cnr-pdr/source/autori:Massimiliano Labardi, Daniele Prevosto, and Simone Capaccioli/titolo:Electrostatic Force Microscopy Techniques for Interphase Characterization/titolo_volume:Hybrid Organic-Inorganic Interfaces: Towards Advanced Functional Materials/curatori_volume:Delville Marie Helene, Taubert Andreas/editore:

/anno:2018

2)-Amorphous fractions of poly(lactic acid)

Righetti M.C.subjectCrystallinitysubjectInterphasesubjectMobile amorphous fractionsubjectrigid amorphpus fraction

Synthesis, Structure and Properties of Poly(lactic acid), edited by Maria Laura Di Lorenzo, René Androsch, pp. 195–234. Berlin: Springer International Publishing AG, 2018

https://dx.doi.org/10.1007/12_2016_14

info:cnr-pdr/source/autori:Righetti M.C./titolo:Amorphous fractions of poly(lactic acid)/titolo_volume:Synthesis, Structure and Properties of Poly(lactic acid)/curatori_volume:Maria Laura Di Lorenzo, René Androsch/editore:

/anno:2018

3)-Analysis of polymer crystallization by calorimetry

M. L. Di Lorenzo; R. Androsch; A. M. Rhoades; M. C. RighettisubjectPolymer crystallizationsubjectcalorimetry

Handbook of Thermal Analysis and Calorimetry: Recent Advances, Techniques and Applications, Volume 6, 2nd Edition, edited by S. Vyazovkin, N. Koga, C. Schick, pp. 253–299. Amsterdam: Elsevier BV, 2018

https://www.sciencedirect.com/science/article/pii/B9780444640628000073?via%3Dihub

info:cnr-pdr/source/autori:M. L. Di Lorenzo, R. Androsch, A. M. Rhoades, M. C. Righetti/titolo:Analysis of polymer crystallization by calorimetry/titolo_volume:Handbook of Thermal Analysis and Calorimetry: Recent Advances, Techniques and Applications, Volume 6, 2nd Edition/curatori_volume:S. Vyazovkin, N. Koga, C. Schick/editore:

/anno:2018

4)-Comparison among nanostructured biomaterials with different mechanisms and kinetics of bioactivity and antibacterial action

Silvia Spriano; Seiji Yamaguchi; Sara Ferraris; Martina Cazzola; MartaMiola; Enrica Vernè; Andrea Cochis; Caterina Cristallini; NiccolettaBarbani; Inger Odnevall Wallinder; Yolanda Hedbergsubjectbioactive materialssubjectsurface functionalizationsubjecttitanium

TERMIS Conference, Kyoto (Japan), 4/7 September 2018

http://www.cnr.it/prodotto/i/397135

info:cnr-pdr/source/autori:Silvia Spriano,Seiji Yamaguchi,Sara Ferraris,Martina Cazzola,Marta Miola,Enrica Vernè,Andrea Cochis,Caterina Cristallini,Niccoletta Barbani,Inger Odnevall Wallinder,Yolanda Hedberg/congresso_nome:TERMIS Conference/congresso_luogo:Kyoto (Japan)/congresso_data:4/7 September 2018/anno:2018/pagina_da:/pagina_a:/intervallo_pagine:

5)-Physical ageing of semi-crystalline PLLA: Role of the differently constrained amorphous fractions

M.C. Righetti; N. Delpouve; A. SaitersubjectPoly(L-lactic acid); Physical ageingsubjectStructural relaxationsubjectConstrained amorphous fraction

TOP Conference 2018, Ischia, 17-21 June 2018

http://www.cnr.it/prodotto/i/397926

info:cnr-pdr/source/autori:M.C. Righetti, N. Delpouve, A. Saiter/congresso_nome:TOP Conference 2018/congresso_luogo:Ischia/congresso_data:17-21 June 2018/anno:2018/pagina_da:/pagina_a:/intervallo_pagine:

6)-Effect of different nucleating agent on crystallinity and properties of polylactic acid

L. Aliotta; P. Cinelli; M.C. Righetti; M.B. Coltelli; A. LazzerisubjectNucleating agentssubjectCrystallinitysubjectMechanical propertiessubjectPoly(lactic acid).

TOP Conference 2018, Ischia, 17-21 June 2018

http://www.cnr.it/prodotto/i/397927

info:cnr-pdr/source/autori:L. Aliotta, P. Cinelli, M.C. Righetti, M.B. Coltelli, A. Lazzeri/congresso_nome:TOP Conference 2018/congresso_luogo:Ischia/congresso_data:17-21 June 2018/anno:2018/pagina_da:/pagina_a:/intervallo_pagine: