Peer-reviewed journal articles

1)-Development and characterization of novel agar and gelatin injectable hydrogel as filler for peripheral nerve guidance channels

Tonda-Turo, Chiara; Gnavi, Sara; Ruini, F.; Gambarotta, Giovanna; Gioffredi, Emilia; Chiono, Valeria; Perroteau, Isabelle; Ciardelli, GianlucasubjectAgarsubjectGelatinsubjectGlial-like cellssubjectHydrogelsubjectInjectablesubjectPeripheral nerve regeneration

Journal of tissue engineering and regenerative medicine (2017).

https://dx.doi.org/10.1002/term.1902

2)-Alumina-supported sub-nanometer Pt-10 clusters: amorphization and role of the support material in a highly active CO oxidation catalyst

Yin, Chunrong; Negreiros, Fabio R.; Barcaro, Giovanni; Beniya, Atsushi; Sementa, Luca; Tyo, Eric C.; Bartling, Stephan; Meiwes-Broer, Karl-Heinz; Seifert, Sonke; Hirata, Hirohito; Isomura, Noritake; Nigam, Sandeep; Majumder, Chiranjib; Watanabe, Yoshihide; Fortunelli, Alessandro; Vajda, Stefansubjectultrananocluster catalystssubjectcarbon oxide oxidation

Journal of Materials Chemistry A 5 (2017): 4923–4931.

https://dx.doi.org/10.1039/c6ta10989f

3)-Au21S(SAdm)(15): An Anisotropic Gold Nanomolecule. Optical and Photoluminescence Spectroscopy and First-Principles Theoretical Analysis

Fortunelli, Alessandro; Sementa, Luca; Thanthirige, Viraj Dhanushka; Jones, Tanya C.; Stener, Mauro; Gagnon, Kevin J.; Dass, Amala; Ramakrishna, Gudasubjectmnolayer protected clusterssubjectoptical spectrumsubjectanisotropic gold clusters

The journal of physical chemistry letters 8 (2017): 457–462.

https://dx.doi.org/10.1021/acs.jpclett.6b02810

4)-Atomistic modelling of Si nanoparticles synthesis

Barcaro G.; Monti S.; Sementa L.; Carravetta V.subjectMolecular dynamicssubjectPlasma synthesissubjectReactive force fieldsubjectSi nanoparticlesubjectTheoretical model

Crystals (Basel) 7 (2017).

https://dx.doi.org/10.3390/cryst7020054

5)-Tuning the functionalization degree of amylose and amylopectin with photochromic spiropyran by CuAAc reaction

David Barsi; Silvia Borsacchi; Lucia Calucci; Antonio Tarantino; Calogero Pinzino; Monica Bertoldosubjectstarchsubjectphotochromic materialssubjectCuAAc

Polymer (Amsterdam. Online) (2017).

https://dx.doi.org/10.1016/j.polymer.2017.05.046

6)-Au21S(SAdm)(15): Crystal Structure, Mass Spectrometry, Optical Spectroscopy, and First-Principles Theoretical Analysis

Jones, Tanya C.; Sementa, Luca; Stener, Mauro; Gagnon, Kevin J.; Thanthirige, Viraj Dhanushka; Ramakrishna, Guda; Fortunelli, Alessandro; Dass, Amalasubjectmonolayer-protected clusterssubjectmetal nanoclusterssubjectoptical responsesubjecttheorysubjectanisotropic nanoclusters
Journal of physical chemistry. C 121 (2017): 10865–10869.
https://dx.doi.org/10.1021/acs.jpcc.6b12075

7)-Ligand-Enhanced Optical Response of Gold Nanomolecules and Its Fragment Projection Analysis: The Case of Au-30(SR)(18)
Sementa, Luca; Barcaro, Giovanni; Baseggio, Oscar; De Vetta, Martina; Dass, Amala; Apra, Edoardo; Stener, Mauro; Fortunelli, Alessandrosubjectmonolayer-protected clusterssubjectmetal nanoclusterssubjectoptical responsesubjectoptical enhancement
Journal of physical chemistry. C 121 (2017): 10832–10842.
https://dx.doi.org/10.1021/acs.jpcc.6b12029

8)-Magnetic Ordering in Gold Nanoclusters
Mikhail Agrachev; Sabrina Antonello; Tiziano Dainese; Marco Ruzzi; Alfonso Zoleo; Edoardo Aprà; Niranjan Govind; Fortunelli, Alessandro; Luca Sementa; Flavio Maransubjectspin-orbit couplingsubjectgold nanoclusterssubjectmonolayer-protected clusters
ACS omega 2 (2017): 2607–2617.
https://dx.doi.org/10.1021/acsomega.7b00472

9)-Parametrizaton of a Reactive Force Field (ReaxFF) for Molecular Dynamics Simulations of Si Nanoparticles.
Barcaro, Giovanni; Monti, Susanna; Sementa, Luca; Carravetta, VincenzosubjectTheory Si nanoparticle REAX
Journal of chemical theory and computation (2017).
https://dx.doi.org/10.1021/acs.jctc.7b00445

10)-Dynamical behavior of microgels of interpenetrated polymer networks.
Nigro, Valentina; Angelini, Roberta; Bertoldo, Monica; Bruni, Fabio; Ricci, Maria Antonietta; Ruzicka, BarbarasubjectPolymer Network
Soft matter (Online) (2017).
https://dx.doi.org/10.1039/c7sm00739f

11)-Highly thermostable and crystalline poly(butylene adipate) bionanocomposites prepared by in situ polycondensation with organically modified Moroccan beidellite clay
Ilsouk, Mohamed; Raihane, Mustapha; Castelvetro, Valter; Lahcini, Mohammed; Bronco, Simona; Rhouta, Benaissa; Bianchi, Sabrina; Conzatti, Luciasubjectbionanocompositessubjectbeidellite claysubjectpoly(butylene adipate)subjectin situ polycondensationsubjectstructure characterizationsubjectthermal properties
Polymer international 66 (2017): 939–949.
https://dx.doi.org/10.1002/pi.5342

12)-Core Size Interconversions of Au-30(S-tBu)(18) and Au-36(SPhX)(24)

Dass, Amala; Jones, Tanya C.; Theivendran, Shevanuja; Sementa, Luca; Fortunelli, AlessandrosubjectPROTECTED GOLD CLUSTERS; RAY CRYSTAL-STRUCTURE; THEORETICAL-ANALYSIS; NANOMOLECULES; THIOLATE; NANOCLUSTERS; AU-144(SCH2CH2PH)(60); TRANSFORMATION; NANOPARTICLES; CONVERSION

Journal of physical chemistry. C 121 (2017): 14914–14919.

https://dx.doi.org/10.1021/acs.jpcc.7b03860

13)-Core-Size Conversion of Au<inf>38</inf>(SCH<inf>2</inf>CH<inf>2</inf>Ph)<inf>24</inf> to Au<inf>30</inf>(S-tBu)<inf>18</inf> Nanomolecules

Rambukwella, Milan; Sementa, Luca; Fortunelli, Alessandro; Dass, AmalasubjectTHEORETICAL-ANALYSIS; CRYSTAL-STRUCTURE; GOLD CLUSTERS; OPTICAL SPECTROSCOPY; NANOPARTICLES; THIOLATE; AU-144(SCH2CH2PH)(60); ELECTROCHEMISTRY; TRANSFORMATION; MOLECULES

Journal of physical chemistry. C 121 (2017): 14929–14935.

https://dx.doi.org/10.1021/acs.jpcc.7b04201

14)-Intense fluorescence of Au-20 (vol 147, 074301, 2017)

Yu, Chongqi; Harbich, Wolfgang; Sementa, Luca; Ghiringhelli, Luca; Apra, Edoardo; Stener, Mauro; Fortunelli, Alessandro; Brune, HaraldsubjectErrata Corrige

The Journal of chemical physics 147 (2017): 5001985.

https://dx.doi.org/10.1063/1.5001985

15)-Intense fluorescence of Au<inf>20</inf>

Yu, Chongqi; Harbich, Wolfgang; Sementa, Luca; Ghiringhelli, Luca; Aprá, Edoardo; Stener, Mauro; Fortunelli, Alessandro; Brune, HaraldsubjectGOLD NANOCLUSTERS; METAL-CLUSTERS; IN-VIVO; NANOPARTICLES; PHOTOLUMINESCENCE; APPROXIMATION; EXCHANGE; MATRICES; ORIGIN; AU2

The Journal of chemical physics 147 (2017): 074301.

https://dx.doi.org/10.1063/1.4996687

16)-Magnetic Ordering in Gold Nanoclusters (vol 2, pg 2607, 2017)

Agrachev, Mikhail; Antonello, Sabrina; Dainese, Tiziano; Ruzzi, Marco; Zoleo, Alfonso; Apra, Edoardo; Govind, Niranjan; Fortunelli, Alessandro; Sementa, Luca; Maran, FlaviosubjectMagnetic Ordering Gold Nanoclusters

ACS omega 2 (2017): 3595–3595.

https://dx.doi.org/10.1021/acsomega.7b00895

17)-High-Field Electron Paramagnetic Resonance Reveals a Stable Glassy Fraction up to Melting in Semicrystalline Poly(dimethylsiloxane)

Massa C.A.; Pizzanelli S.; Bercu V.; Pardi L.; Leporini D.subjecthigh-field electron paramagnetic resonance (HF-EPR)
Applied magnetic resonance 48 (2017): 827–840.
https://dx.doi.org/10.1007/s00723-017-0903-z

18)-Local Reversible Melting in Semicrystalline Poly(dimethylsiloxane): A High-Field Electron Paramagnetic Resonance Study
Massa C.A.; Pizzanelli S.; Bercu V.; Pardi L.; Leporini D.subjecthigh-field electron paramagnetic resonance (HF-EPR)
Macromolecules (Online) 50 (2017): 5061–5073.
https://dx.doi.org/10.1021/acs.macromol.7b00627

19)-Dynamics and self-assembly of bio-functionalized gold nanoparticles in solution: Reactive molecular dynamics simulations
Monti S.; Barcaro G.; Sementa L.; Carravetta V.; Agren H.subjectbiocompatibilitysubjectcross-linkingsubjectfunctionalizationsubjectnanoparticlesubjectReaxFF
Nano research (Online) (2017): 1–11.
https://dx.doi.org/10.1007/s12274-017-1704-2

20)-Characterization of the adsorption dynamics of trisodium citrate on gold in water solution
Susanna Monti 1; Giovanni Barcaro 2; Luca Sementa 2; Vincenzo Carravetta 2; Hans Ågren 3subjectcitric acidsubjectAuNP stabilizationsubjectReactive Force FieldsubjectSurface adsorption
RSC advances 7 (2017): 49655–49663.
https://dx.doi.org/10.1039/c7ra10759e

21)-Swelling of responsive-microgels: experiments versus models
Valentina Nigro; Roberta Angelini; Monica Bertoldo; Barbara RuzickasubjectColloidal dispersionssubjectMicrogelssubjectSwelling behaviorsubjectDynamic light scattering
Colloids and surfaces. A, Physicochemical and engineering aspects (Print) 532 (2017): 389–396.
https://dx.doi.org/10.1016/j.colsurfa.2017.04.059

22)-Contribution of the rigid amorphous fraction to physical ageing of semi-crystalline PLLA
Righetti, Maria Cristina; Gazzano, Massimo; Delpouve, Nicolas; Saiter, AllissonsubjectCrystallinitysubjectMobile amorphous fractionsubjectRigid amorphous fractionsubjectInterphasesubjectStructural relaxation
Polymer (Guildford) 125 (2017): 241–253.
https://dx.doi.org/10.1016/j.polymer.2017.07.089

23)-Effect of nucleating agents on crystallinity and properties of poly (lactic acid) (PTA)

Aliotta, Laura; Cinelli, Patrizia; Coltelli, Maria Beatrice; Righetti, Maria Cristina; Gazzano, Massimo; Lazzeri, AndreasubjectPoly(lactic acid)subjectNucleating agentsubjectMechanical propertiessubjectTakayanagi modelsubjectCrystallinity phases
European Polymer Journal 93 (2017): 822–832.
https://dx.doi.org/10.1016/j.eurpolymj.2017.04.041

24)-Low-temperature crystallization of poly(butylene succinate)
Di Lorenzo, Maria Laura; Androsch, Rene; Righetti, Maria CristinasubjectPolymer crystallizationsubjectPoly(butylene succinate)subjectThermal analysis
European Polymer Journal 94 (2017): 384–391.
https://dx.doi.org/10.1016/j.eurpolymj.2017.07.025

25)-Nonadiabatic Renner-Teller quantum dynamics of OH(X-2 Pi) + H+ reactive collisions
Gamallo, Pablo; Akpinar, Sinan; Defazio, Paolo; Petrongolo, Carlosubjectdinamica molecolare quantistica non adiabatica
PCCP. Physical chemistry chemical physics (Print) 19 (2017): 4454–4461.
https://dx.doi.org/10.1039/c6cp07756k

26)-Dynamics of poly(vinyl butyral) studied using dielectric spectroscopy and 1H NMR relaxometry
S. Pizzanelli; D. Prevosto; M. Labardi; T. Guazzini; S. Bronco; C. Forte; L. Caluccisubjectpoly(vinyl butyral) dielectric spectroscopy NMR relaxometry
Physical chemistry chemical physics (Online) 19 (2017): 31804.
https://dx.doi.org/10.1039/c7cp02595e

27)-Direct Evidence of Relaxation Anisotropy Resolved by High Pressure in a Rigid and Planar Glass Former
Tu; Wenkang; Valenti; Sofia; Ngai; K. L.; Capaccioli; Simone; Liu; Ying Dan; Wang; Li-MinsubjectSECONDARY RELAXATION; FORMING SYSTEMS; METALLIC-GLASS; IONIC LIQUID; TRANSITION; DYNAMICS; TOLUENE; TEMPERATURE; CRYSTALS; CLUSTERS
The journal of physical chemistry letters 8 (2017): 4341–4346.
https://dx.doi.org/10.1021/acs.jpclett.7b01837

28)-Design and development of a hybrid bioartificial water-induced shape memory polymeric material as an integral component for the anastomosis of human hollow organs
Paonessa S.; Barbani N.; Rocchietti E.C.; Giachino C.; Cristallini C.subjectBowel; Anastomosis; Hydrogels; Poly(vinyl alcohol); Acetylsalicylic acid
Materials science & engineering. C, Biomimetic materials, sensors and systems (Print) 75 (2017): 1427–1434.
https://dx.doi.org/10.1016/j.msec.2017.03.039

29)-Critical structural fluctuations of proteins upon thermal unfolding challenge the Lindemann criterion

Katava; Marina; Stirnemann; Guillaume; Zanatta; Marco; Capaccioli; Simone; Pachetti; Maria; Ngai; K. L.; Sterpone; Fabio; Paciaroni; Alessandrosubjectneutron scattering; molecular dynamics simulation; protein dynamics; Lindemann criterion; cell thermal stability

Proceedings of the National Academy of Sciences of the United States of America 114 (2017): 9361–9366.

https://dx.doi.org/10.1073/pnas.1707357114

30)-Quantitative explanation of the enhancement of surface mobility of the metallic glass Pd40Cu30Ni10P20 by the Coupling Model

Ngai; K. L.; Capaccioli; S.; Cao; C. R.; Bai; H. Y.; Wang; W. H.subjectMetallic glass; Surface diffusion; Coupling model

Journal of non-crystalline solids 463 (2017): 85–89.

https://dx.doi.org/10.1016/j.jnoncrysol.2017.03.002

31)-Dynamics of hydrated proteins and bio-protectants: Caged dynamics, beta-relaxation, and alpha-relaxation

Ngai; K. L.; Capaccioli; S.; Paciaroni; A.subjectHydrated protein dynamics; Neutron scattering; Protein dynamical transition; Secondary relaxation of hydration water; Myoglobin; Lysozyme; Bovine serum albumin; Bio-protectants

Biochimica et biophysica acta. G, General subjects (Print) 1861 (2017): 3553–3563.

https://dx.doi.org/10.1016/j.bbagen.2016.04.027

32)-Molecularly imprinted polymers by phase inversion technique for the selective recognition of saccharides of biomedical interest in aqueous solutionsMolecularly imprinted polymers by phase inversion technique for the selective recognition of saccharides of biomedical interest in aqueous solutions

Niccoletta Barbani; Elisabetta Rosellini; Marco Donati; Paolo Costantino; Caterina Cristallini; Gianluca CiardellisubjectD-manno-octulosonate; vaccine purification

Polymer international (Online) 66 (2017): 900–907.

https://dx.doi.org/10.1002/pi.5334

33)-Design, fabrication and characterization of composite piezoelectric ultrafine fibers for cochlear stimulation

Mota, Carlos; Labardi, Massimiliano; Trombi, Luisa; Astolfi, Laura; D'Acunto, Mario; Puppi, Dario; Gallone, Giuseppe; Chiellini, Federica; Berrettini, Stefano; Bruschini, Luca; Danti, SerenasubjectElectrospinningsubjectBarium titanatesubjectPolyvinylidene fluoridesubjectAligned fiberssubjectNeural cellssubjectTransducer

Materials & design 122 (2017): 206–219.

https://dx.doi.org/10.1016/j.matdes.2017.03.013

34)-Crystallization of Polymers Investigated by Temperature-Modulated DSC

Righetti; Maria Cristinasubjectpolymersubjectcrystallizationsubjectdifferential scanning calorimetrysubjecttemperature-modulated differential scanning calorimetrysubjectreversing meltingsubjectreversible meltingsubjectcrystalline fractionsubjectmobile amorphous fractionsubjectrigid amorphous fraction
Materials (Basel) 10 (2017).
https://dx.doi.org/10.3390/ma10040442

35)-Endothermic features on heating of glasses show that the second glass to liquid transition of water was phenomenologically-mistaken
Righetti, Maria Cristina; Tombari, Elpidio; Johari, G. P.subjectGlass transitionsubjectWatersubjectPolymersubjectGlass phenomenology
Thermochimica Acta 647 (2017): 101–110.
https://dx.doi.org/10.1016/j.tca.2016.11.011

36)-A push-pull silafluorene fluorophore for highly efficient luminescent solar concentrators
Gianfaldoni, Federico; De Nisi, Francesca; Iasilli, Giuseppe; Panniello, Annamaria; Fanizza, Elisabetta; Striccoli, Marinella; Ryuse, Daiki; Shimizu, Masaki; Biver, Tarita; Pucci, Andreasubjectsolar concentratorssubjectFluorophores
RSC advances 7 (2017): 37302–37309.
https://dx.doi.org/10.1039/c7ra08022k

37)-Ultrasound-activated piezoelectric P(VDF-TrFE)/boron nitride nanotube composite films promote differentiation of human SaOS-2 osteoblast-like cells
Genchi G.G.; Sinibaldi E.; Ceseracciu L.; Labardi M.; Marino A.; Marras S.; De Simoni G.; Mattoli V.; Ciofani G.subjectBonesubjectBoron nitride nanotubessubjectCell differentiationsubjectP(VDF-TrFE)subjectPiezoelectricitysubjectUltrasounds
Nanomedicine (Online) 14 (2017): 2421–2432.
https://dx.doi.org/10.1016/j.nano.2017.05.006

38)-Ab initio modelling of oxygen vacancy arrangement in highly defective HfO2 resistive layers
Sementa; Luca; Larcher; Luca; Barcaro; Giovanni; Montorsi; MoniasubjectMEMORYsubjectRRAM; DYNAMICS
PCCP. Physical chemistry chemical physics (Print) 19 (2017): 11318–11325.
https://dx.doi.org/10.1039/c7cp01216k

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

1)-Electronic Structure of Oxide Ultrathin Layers on Metal Surfaces

Barcaro, Giovanni; Fortunelli, AlessandrosubjectBand gapsubjectDensity functional theory (DFT)subjectDensity of statessubjectHubbard HamiltoniansubjectMetallizationsubjectPolaritysubjectReducible oxidesubjectRumplingsubjectStoichiometry StructuresubjectSurface dipolesubjectWork function
Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, 2017, edited by Klaus Wandelt. Amsterdam: Elsevier, 2017
https://dx.doi.org/10.1016/B978-0-12-409547-2.12887-2

info:cnr-pdr/source/autori:Barcaro, Giovanni; Fortunelli, Alessandro/titolo:Electronic Structure of Oxide Ultrathin Layers on Metal Surfaces/titolo_volume:Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, 2017/curatori_volume:Klaus Wandelt/editore:

/anno:2017

2)-DYNAMICS OF POLY(VINYL BUTYRAL) STUDIED BY DIELECTRIC SPECTROSCOPY AND 1H NMR RELAXOMETRY

Silvia Pizzanelli; Daniele Prevosto; Massimiliano Labardi; Tommaso Guazzini; Simona Bronco; Claudia Forte; Lucia Caluccisubjectpoly(vinyl butyral)subjectdielectric spectroscopysubject1H NMR FFC relaxometry
XLVI national Congress on Magnetic Resonance, Fisciano (Salerno), 27-29/09/2017
http://www.cnr.it/prodotto/i/376368

info:cnr-pdr/source/autori:Silvia Pizzanelli, Daniele Prevosto, Massimiliano Labardi, Tommaso Guazzini, Simona Bronco, Claudia Forte, Lucia Calucci/congresso_nome:XLVI national Congress on Magnetic Resonance/congresso_luogo:Fisciano (Salerno)/congresso_data:27-29/09/2017/anno:2017/pagina_da:/pagina_a:/intervallo_pagine:

3)-Polymer dynamics and morphology in LDPE nanocomposites studied by NMR spectroscopy and relaxometry

PIZZANELLI, Silvia; CALUCCI, Lucia; MASSA, Carlo Andrea; FORTE, ClaudiasubjectLDPEsubjectsolid state NMRsubjectNMR relaxometrysubjectnanocomposite
Multiscale phenomena in molecular matter, Cracovia, 3-6/07/2017
http://www.cnr.it/prodotto/i/376366

info:cnr-pdr/source/autori:PIZZANELLI, Silvia; CALUCCI, Lucia; MASSA, Carlo Andrea; FORTE, Claudia/congresso_nome:Multiscale phenomena in molecular

matter/congresso_luogo:Cracovia/congresso_data:3-6/07/2017/anno:2017/pagina_da:/pagina_a:/intervallo_pagine:

4)-Reductive Amination Vs "Click" Reaction On The Grafting Of Polysaccharides Onto Janus Silica

D. Barsi; A. Bianchi; M. Corricelli; M. L. Curri; A. Farah; M. BertoldosubjectnanomaterialssubjectJanus particlessubjectpolysaccharides
European Polymer Conference 2017, Lione (Fr), 02/07/2017, 07/07/2017
http://www.cnr.it/prodotto/i/377521

info:cnr-pdr/source/autori:D. Barsi; A. Bianchi; M. Corricelli; M. L. Curri; A. Farah; M. Bertoldo/congresso_nome:European Polymer Conference 2017/congresso_luogo:Lione (Fr)/congresso_data:02/07/2017, 07/07/2017/anno:2017/pagina_da:/pagina_a:/intervallo_pagine:

5)-Thermodynamic and dynamic of concentrated PNIPAM microgels

Elena Burattia; Andrea Orecchini; Marco Zanatta; Emanuela Zaccarelli; Monica BertoldosubjectMicrogelssubjectneutron scatteringsubjectDSC
European Polymer Conference 2017 (EPF 2017), Lyon, 02/07/2017, 07/07/2017
http://www.cnr.it/prodotto/i/377522

info:cnr-pdr/source/autori:Elena Burattia; Andrea Orecchini; Marco Zanatta; Emanuela Zaccarelli; Monica Bertoldo/congresso_nome:European Polymer Conference 2017 (EPF 2017)/congresso_luogo:Lyon/congresso_data:02/07/2017, 07/07/2017/anno:2017/pagina_da:/pagina_a:/intervallo_pagine: