Peer-reviewed journal articles

1)-Two-dimensional iron oxide bi-and trilayer structures on Pd(100)

Kuhness, D.; Pomp, S.; Mankad, V.; Barcaro, G.; Sementa, L.; Fortunelli, A.; Netzer, F. P.; Surnev, S.SUBJECTDFTSUBJECTIron oxide filmSUBJECTLEEDSUBJECTSTMSUBJECTXASSUBJECTXPS

Surface science 645 (2016): 13–22.

https://dx.doi.org/10.1016/j.susc.2015.10.032

2)-Ab initio study of the enantio-selective magnetic-field-induced second harmonic generation in chiral molecules

A. Rizzo; G. L. D. J. Rikken; R. MathevetSUBJECTNonlinear optical properties; Magnetic Field; SHG

Physical Chemistry Chemical Physics 18 (2016): 1846–1858.

https://dx.doi.org/10.1039/c5cp07127e

3)-Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic Properties of the D102 Indoline Dye on an Anatase (101) Substrate

Monti, Susanna; Pastore, Mariachiara; Li, Cui; De Angelis, De Angelis, Filippo; Carravetta, VincenzoSUBJECTD102 Indoline Dye on an Anatase

Journal of physical chemistry. C 120 (2016): 2787–2796.

https://dx.doi.org/10.1021/acs.jpcc.5b11332

4)-Origin-independent two-photon circular dichroism calculations in coupled cluster theory.

D. H. Friese; C. Hattig; A. RizzoSUBJECTTwo-photon SpectroscopySUBJECTCircular DichroismSUBJECTComputational ModelSUBJECTCoupled Cluster TheorySUBJECTNonlinear Spectroscopy

Physical chemistry chemical physics (Online) 18 (2016): 13689–13692.

https://dx.doi.org/10.1039/c6cp01653g

5)-A complex-polarization-propagator magneto-chiral axial dichroism and dispersion

J. Cukras; J. Kauczor; P. Norman; A. Rizzo; G. L. J. A. Rikken; S. CorianiSUBJECTMagnetochiralitySUBJECTAxial DichroismSUBJECTAxial BirefringenceSUBJECTComputational ProtocolSUBJECTComplex Polarization Propagator

Physical chemistry chemical physics (Online) 18 (2016): 13267–13279.

https://dx.doi.org/10.1039/C6CP01465H

6)-Experimental and theoretical XPS and NEXAFS studies of N-methylacetamide and N-methyltrifluoroacetamide

Li, Cui; Salen, Peter; Yatsyna, Vasyl; Schio, Luca; Feifel, Raimund; Squibb, Richard; Kaminska, Magdalena; Larsson, Mats; Richter, Robert; Alagia, Michele; Stranges, Stefano; Monti, Susanna; Carravetta, Vincenzo; Zhaunerchyk,

VitaliSUBJECTexperimentSUBJECTtheorySUBJECTXPSSUBJECTNEXAFSSUBJECTN-methylacetamideSUBJECTN-methyltrifluoroacetamide
PCCP. Physical chemistry chemical physics (Print) 18 (2016): 2210–2218.
https://dx.doi.org/10.1039/c5cp06441d

7)-Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics
Monti, Susanna; Carravetta, Vincenzo; Agren, HansSUBJECTtheorySUBJECTquantum molecular dynamicsSUBJECTgold surfaceSUBJECTcysteine
The journal of physical chemistry letters 7 (2016): 272–276.
https://dx.doi.org/10.1021/acs.jpclett.5b02769

8)-Theoretical study of para-nitro-aniline adsorption on the Au(111) surface
Li, Cui; Monti, Susanna; Li, Xin; Rinkevicius, Zilvinas; Ågren, Hans; Carravetta, VincenzoSUBJECTAu(111)SUBJECTPara-nitro-anilineSUBJECTPNASUBJECTQuantum molecular dynamicsSUBJECTSurface adsorptionSUBJECTX-ray computational spectroscopy
Surface science 649 (2016): 124–132.
https://dx.doi.org/10.1016/j.susc.2016.01.008

9)-The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves
An, Qi; Qian, Jin; Nielsen, Robert R.; Sementa, Luca; Barcaro, Giovanni; Negreiros, Fabio R.; Fortunelli, Alessandro; Goddard, William A., IIISUBJECTsurface acoustic waves - ab initio simulations
Journal of Materials Chemistry A 4 (2016): 12036–12045.
https://dx.doi.org/10.1039/c6ta03669d

10)-Lattice Strain Defects in a Ceria Nanolayer
Ma, Liying; Doudin, Nassar; Surnev, Svetlozar; Barcaro, Giovanni; Sementa, Luca; Fortunelli, Alessandro; Netzer, Falko P.SUBJECTcerium oxide - density functional theory - modeling
The journal of physical chemistry letters 7 (2016): 1303–1309.
https://dx.doi.org/10.1021/acs.jpclett.6b00253

11)-Crystal Structure and Theoretical Analysis of Green Gold Au-30(S-tBu)(18) Nanomolecules and Their Relation to Au30S(S-tBu)(18)
Dass, Amala; Jones, Tanya; Rambukwella, Milan; Crasto, David; Gagnon, Kevin J.; Sementa, Luca; De Vetta, Martina; Baseggio, Oscar; Apra, Edoardo; Stener, Mauro; Fortunelli, AlessandroSUBJECTdensity functional theory - modeling - theoretical design
Journal of physical chemistry. C 120 (2016): 6256–6261.
https://dx.doi.org/10.1021/acs.jpcc.6b00062

12)-Two-Dimensional Iron Tungstate: A Ternary Oxide Layer with Honeycomb Geometry

Pomp, S.; Kuhness, D.; Barcaro, G.; Sementa, L.; Mankad, V.; Mankad, V.; Fortunelli, A.; Sterrer, M.; Netzer, F. P.; Surnev, S.SUBJECTUltrathin oxides - theoretical modeling
Journal of physical chemistry. C 120 (2016): 7629–7638.
https://dx.doi.org/10.1021/acs.jpcc.6b01086

13)-Decoration of gold nanoparticles with cysteine in solution: reactive molecular dynamics simulations
S. Monti; V. Carravetta; H. AgrenSUBJECThybrid materialsSUBJECTnanoparticles decorationSUBJECTfunctionalization
Nanoscale (Print) 8 (2016): 12929–12938.
https://dx.doi.org/10.1039/c6nr03181a

14)-Optical properties of gold nanoclusters functionalized with a small organic compound: Modeling by an integrated quantum-classical approach
Li X.; Carravetta V.; Li C.; Monti S.; Rinkevicius Z.; Agren H.SUBJECTphysisorption on goldSUBJECTsurface adsorptionSUBJECTReaxFFSUBJECTreactive molecular dynamics
Journal of chemical theory and computation 12 (2016): 3325–3339.
https://dx.doi.org/10.1021/acs.jctc.6b00283

15)-Rigid amorphous fraction and multiple melting behavior in poly(butylene terephthalate) and isotactic polystyrene
Righetti, Maria Cristina; Di Lorenzo, Maria LauraSUBJECTCrystallinitySUBJECTInterphaseSUBJECTMelting behaviorSUBJECTRigid amorphous fraction
Journal of thermal analysis and calorimetry (Print) 126 (2016): 521–530.
https://dx.doi.org/10.1007/s10973-016-5553-0

16)-Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative
Liu Y.; Cerezo J.; Santoro F.; Rizzo A.; Lin N.; Zhao X.SUBJECTtheoretical chemistry; photon absorption line-shape; carbazoles
PCCP. Physical chemistry chemical physics (Print) 18 (2016): 22889–22905.
https://dx.doi.org/10.1039/c6cp04162k

17)-Physico-chemical properties of quartz from industrial manufacturing and its cytotoxic effects on alveolar macrophages: The case of green sand mould casting for iron production.
Di Benedetto F.[1,2], Gazzano E.[3,4],Tomatis M.; [4,5], Turci F.[4,5], Pardi L.A.[6], Bronco S.[6], Fornaciai G.[7], Innocenti M.[7], Montegrossi G.[2], Muniz Miranda M.[7], Zoleo A.[8], Capacci F.[9], Fubini B.[5,6], Ghigo D.[3,4], Romanelli M.[1]SUBJECTCarbon coatingSUBJECTCytotoxicitySUBJECTEPR/ESEEMSUBJECTFree radicalsSUBJECTHealth effectsSUBJECTHole and Al centresSUBJECTMacrophagesSUBJECTNOSUBJECTQuartzSUBJECTROS

Journal of hazardous materials (Print) 312 (2016): 18–27.
https://dx.doi.org/10.1016/j.jhazmat.2016.03.016

18)-Recyclability of PET/WPI/PE Multilayer Films by Removal of Whey Protein Isolate-Based Coatings with Enzymatic Detergents

Cinelli, Patrizia; Schmid, Markus; Bugnicourt, Elodie; Coltelli, Maria Beatrice; Lazzeri, AndreaSUBJECTwhey protein isolateSUBJECTenzymatic detergentsSUBJECTrecyclabilitySUBJECTproteaseSUBJECTmultilayer filmsSUBJECTpolyethylene terephthalate (PET)SUBJECTpolyethylene (PE)
Materials (Basel) 9 (2016): 1–15.
https://dx.doi.org/10.3390/ma9060473

19)-Nanoscale Domain Structure and Defects in a 2-D WO3 Layer on Pd(100)

Doudin, N.; Kuhness, D.; Blatnik, M.; Barcaro, G.; Negreiros, F. R.; Sementa, L.; Fortunelli, A.; Surnev, S.; Netzer, F. P.SUBJECT2D oxide - tungsten oxide - computational modeling
Journal of physical chemistry. C 120 (2016): 28682–28693.
https://dx.doi.org/10.1021/acs.jpcc.6b10504

20)-SERS Amplification from Self-Organized Arrays of Plasmonic Nanocrescents

Giordano, Maria Caterina; Foti, Antonino; Foti, Antonino; Messina, Elena; Gucciardi, Pietro Giuseppe; Comoretto, Davide; Buatier De Mongeot, FrancescoSUBJECTbiosensingSUBJECTnanophotonicsSUBJECTnanostructuresSUBJECTplasmonic nanoantennasSUBJECTpolymer nanosphere arraysSUBJECTsurface-enhanced Raman scattering
ACS applied materials & interfaces (Print) 8 (2016): 6629–6638.
https://dx.doi.org/10.1021/acsami.5b11843

21)-Emulsion Blending Approach for the Preparation of Gelatin/Poly(butylene succinate-co-adipate) Films

Bertoldo, Monica; Coltelli, Maria-Beatrice; Messina, Tiziana; Bronco, Simona; Castelvetro, ValterSUBJECTgelatinSUBJECTpoly(butylene succinate-co-adipate)SUBJECTemulsionSUBJECTblendSUBJECTfilmSUBJECTwet processing
ACS biomaterials science & engineering 2 (2016): 677–686.
https://dx.doi.org/10.1021/acsbiomaterials.6b00050

22)-Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution

S. Monti; V. Carravetta; H. AgrenSUBJECThybrid materialsSUBJECTgold nanoparticle stabilizationSUBJECTpeptide-metal bindingSUBJECTbiocompatibility
Small (Weinh., Print) (2016).
https://dx.doi.org/10.1002/smll.201602275

23)-P(VDF-TrFE)/BaTiO3 Nanoparticle Composite Films Mediate Piezoelectric Stimulation and Promote Differentiation of SH-SY5Y Neuroblastoma Cells

Genchi, Giada Graziana; Ceseracciu, Luca; Marino, Attilio; Labardi, Massimiliano; Marras, Sergio; Pignatelli, Francesca; Bruschini, Luca; Mattoli, Virgilio; Ciofani, GianniSUBJECTP(VDF-TrFE)SUBJECTpiezoelectricSUBJECTNanoparticle

Advanced healthcare materials (Print) 5 (2016): 1808–1820.

https://dx.doi.org/10.1002/adhm.201600245

24)-Time and Temperature Evolution of the Rigid Amorphous Fraction and Differently Constrained Amorphous Fractions in PLLA

Righetti, Maria Cristina; Prevosto, Daniele; Tombari, ElpidioSUBJECTconstrained mobile amorphous fractionSUBJECTcrystallinitySUBJECTdifferential scanning calorimetry (DSC)SUBJECTinterfacesSUBJECTrigid amorphous fraction

Macromolecular chemistry and physics (Print) 217 (2016): 2013–2026.

https://dx.doi.org/10.1002/macp.201600210

25)-Aging kinetics of levoglucosan orientational glass as a rate dispersion process and consequences for the heterogeneous dynamics view

Righetti, Maria Cristina; Tombari, Elpidio; Johari, G. P.SUBJECTaging

The Journal of chemical physics 145 (2016).

https://dx.doi.org/10.1063/1.4959806

26)-Rod-coil block copolymer as nanostructuring compatibilizer for efficient CdSe NCs/PCPDTBT hybrid solar cells

Zappia, Stefania; Di Mauro, A. Evelyn; Mastria, Rosanna; Rizzo, Aurora; Curri, M. Lucia; Striccoli, Marinella; Destri, SilviaSUBJECTBlock copolymerSUBJECTHybrid solar cellsSUBJECTCdSe nanocrystalsSUBJECTMorphologySUBJECTCompatibilizerSUBJECTAnnealing

European Polymer Journal 78 (2016): 352–363.

https://dx.doi.org/10.1016/j.eurpolymj.2016.03.021

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

1)-Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces

Barcaro, Giovanni; Sementa, Luca; Negreiros, Fabio Ribeiro; Thomas, Iorwerth Owain; Vajda, Stefan; Fortunelli, AlessandroSUBJECT2d materials - theoretical modeling

Oxide Materials at the Two-Dimensional Limit, edited by Alessandro Fortunelli; Falko Netzer, pp. 39–90, 2016

https://dx.doi.org/10.1007/978-3-319-28332-6_2

info:cnr-pdr/source/autori:Barcaro, Giovanni; Sementa, Luca; Negreiros, Fabio Ribeiro; Thomas, Iorwerth Owain; Vajda, Stefan; Fortunelli, Alessandro/titolo:Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces/titolo_volume:Oxide Materials at the Two-Dimensional Limit/curatori_volume:Alessandro Fortunelli; Falko Netzer/editore:/anno:2016

2)-Simulation of physisorption and chemisorption of cysteine on gold substrates in water solutions: classical molecular dynamics based on a reactive force field (ReaxFF)

Monti Susanna; Carravetta Vincenzo; Agren HansSUBJECTfunctionalization of Au surfaces

Multiscale Modelling of Materials and Molecules 2016, pp. 11–11, Uppsala, 7-9 june 2016

http://www.cnr.it/prodotto/i/358900

info:cnr-pdr/source/autori:Monti Susanna, Carravetta Vincenzo, Agren Hans/congresso_nome:Multiscale Modelling of Materials and Molecules 2016/congresso_luogo:Uppsala/congresso_data:7-9 june 2016/anno:2016/pagina_da:11/pagina_a:11/intervallo_pagine:11–11

3)-Kinetic quasimodes in a plasma double layer

Nocera L.SUBJECTVlasov equationSUBJECTLiouville operatorSUBJECTSpectral representationSUBJECTGreen functionSUBJECTSurfce waves

102nd National Congress of the Italian Physical Society, pp. 218–218, Padova, 26-30 September 2016

urn:isbn:978-88-7438-106-7

info:cnr-pdr/source/autori:Nocera L./congresso_nome:102nd National Congress of the Italian Physical Society/congresso_luogo:Padova/congresso_data:26-30 September 2016/anno:2016/pagina_da:218/pagina_a:218/intervallo_pagine:218–218

4)-INVESTIGATION OF POLYMER DYNAMICS IN PVB-ATO NANOCOMPOSITES BY LOW-FIELD AND FAST FIELD-CYCLING 1H NMR RELAXOMETRY

Silvia Pizzanelli; Lucia Calucci; Claudia Forte; Simona Bronco; Chiara Serraglini; Tommaso GuazziniSUBJECTATOSUBJECTPVBSUBJECTNanocompositesSUBJECTNMR relaxometry

XLV NATIONAL CONGRESS ON MAGNETIC RESONANCE Frontiers of Nuclear Magnetic Resonance: Translational Aspects and Advanced Solutions to New Scientific, Technological, and Societal Challenges, Modena, 05-07/09/2016
http://www.cnr.it/prodotto/i/359703

info:cnr-pdr/source/autori:Silvia Pizzanelli, Lucia Calucci, Claudia Forte, Simona Bronco, Chiara Serraglini, Tommaso Guazzini/congresso_nome:XLV NATIONAL CONGRESS ON MAGNETIC RESONANCE Frontiers of Nuclear Magnetic Resonance: Translational Aspects and Advanced Solutions to New Scientific, Technological, and Societal Challenges/congresso_luogo:Modena/congresso_data:05-07/09/2016/anno:2016/pagina_da:/pagina_a:/intervallo_pagine: