

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 filmssubjectLEEDsubjectSTMsubjectXASsubjectXPS
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 Models subjectCoupled 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. CorianisubjectMagneto-chiralitysubjectAxial DichroismsubjectAxial BirefringencesubjectComputational Protocols subjectComplex 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.jpcllett.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.jpcllett.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 decorationssubjectfunctionalization
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, Francescosubjectbiosensingsubjectnanophotonicssubjectnanostructuresubjectplasmonic 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/sml.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, Gianni
subjectP(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, Elpidio
subjectconstrained mobile amorphous fractions
subjectcrystallinitysubjectdifferential 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, Silvia
subjectBlock 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, Alessandro
subject 2d 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 Hans
subject functionalization 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.
subject Vlasov equations subject Liouville operators subject Spectral representations subject Green functions subject Surface 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 Guazzini
subject ATO subject PVB subject Nanocomposites subject NMR 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: