

Publications

1 Chain dynamics on crossing the glass transition: nonequilibrium effects and recovery of the temperature dependence of the structural relaxation.

Arrese-Igor S, Alegria A, and Colmenero J.
ACS Macro Letters 3, 1215 (2014).

2 Cluster glasses of semiflexible ring polymer.

Slimani MZ, Bacova P, Bernabei M, Narros A, Likos CN, and Moreno AJ.
ACS Macro Letters 3, 611 (2014).

3 How far are single-chain polymer nanoparticles in solution from the globular state?

Pomposo JA, Perez-Baena I, Lo Verso F, Moreno AJ, Arbe A, and Colmenero J.
ACS Macro Letters 3, 767 (2014).

4 Metallo-folded single-chain nanoparticles with catalytic selectivity.

Sanchez-Sanchez A, Arbe A, Colmenero J, and Pomposo JA.
ACS Macroletters 3, 439 (2014).

5 Epitaxially connected PbSe quantum-dot films: controlled neck formation and optoelectronic properties.

Sandeep CSS, Azpiroz JM, Evers WH, Boehme SC, Moreels I, Kinge S, Siebbeles LDA, Infante I, and Houtepen AJ.
ACS Nano 8, 11499 (2014).

6 Spectroscopic fingerprints of work-function-controlled phthalocyanine charging on metal surfaces.

Borghetti P, Ei-Sayed A, Goiri E, Rogero C, Lobo-Checa J, Floreano L, Ortega JE, and de Oteyza DG.
ACS Nano 8, 12786 (2014).

7 Revealing the adsorption mechanisms of nitroxides on ultrapure, metallicity-sorted carbon nanotubes.

Ruiz-Soria G, Paz AP, Sauer M, Mowbray DJ, Lacovig P, Dalmiglio M, Lizzit S, Yanagi K, Rubio A, Goldoni A, Ayala P, and Pichler T.
ACS Nano 8, 1375 (2014).

8 Electrochemical control over photoinduced electron transfer and trapping in CdSe-CdTe quantum-dot solids.

Boehme SC, Walvis TA, Infante I, Grozema FC, Vanmaekelbergh D, Siebbeles LDA, and Houtepen AJ. ACS NANO 8, 7067 (2014).

9 Luminescence, patterned metallic regions, and photon-mediated electronic changes in single-sided fluorinated graphene sheets.

Walter AL, Sahin H, Jeon KJ, Bostwick A, Horzum S, Koch R, Speck F, Ostler M, Nagel P, Merz M, Schupler S, Moreschini L, Chang YJ, Seyller T, Peeters FM, Horn K, and Rotenberg E. ACS NANO 8, 7801 (2014).

10 Lasing threshold of one- and two-photon-pumped dye-doped silica powder.

Garcia-Ramiro B, Illarramendi MA, Garcia-Revilla S, Balda R, Levy D, Zayat M, and Fernandez J. Applied Physics B-Lasers and Optics 117, 1135 (2014).

11 Photo-induced strengthening of weak bonding in noble gas dimers.

Miyamoto Y, Miyazaki T, Rubio A, and Zhang H. Applied Physics Letters 104, 201107 (2014).

12 Modeling anisotropic plasmon excitations in self-assembled fullerenes.

Iurov A, Gumbs G, Gao B, and Huang D. Applied Physics Letters 104, 203103 (2014).

13 Proposal for a phase-coherent thermoelectric transistor.

Giazotto F, Robinson JWA, Moodera JS, and Bergeret FS. Applied Physics Letters 105, 062602 (2014).

14 Proximity nanovalve with large phase-tunable thermal conductance.

Strambini E, Bergeret FS, and Giazotto F. Applied Physics Letters 105, 082601 (2014).

15 VLT/AMBER observations of cold giant stars: atmospheric structures and fundamental parameters.

Arroyo-Torres B, Marti-Vidal I, Marcaide JM, Wittkowski M, Guirado JC, Hauschildt PH, Quirrenbach A, and Fabregat J. Astronomy and Astrophysics 566, A88 (2014).

16 Constraints on the progenitor system and the environs of SN 2014J from deep radio observations.

Perez-Torres MA, Lundqvist P, Beswick RJ, Bjornsson CI, Muxlow TWB, Paragi Z, Ryder S, Alberdi A, Fransson C, Marcaide JM, Marti-Vidal I, Ros E, Argo MK, and Guirado JC. Astrophysical Journal 792, 38 (2014).

17 Spectral and morphological analysis of the remnant of supernova 1987 a with alma and atca.

Zanardo G, Staveley-Smith L, Indebetouw R, Chevalier RA, Matsuura M, Gaensler BM, Barlow MJ, Fransson C, Manchester RN, Baes M, Mamenetzky JR, Lakicevic M, Lundqvist P, Marcaide JM, Marti-Vidal I, Meixne M, Ng CY, Park S, Sonneborn G, Spyromilio J, and van Loon JT. Astrophysical Journal 796, 82 (2014).

18 Could the lithium bond be classified as the r-hole bond? – QTAIM and NBO analysis.

Lipkowski P, and Grabowski SJ. Chemical Physics Letters 591, 113 (2014).

19 Halogen bond with the multivalent halogen acting as the Lewis acid center.

Grabowski SJ. Chemical Physics Letters 605, 131 (2014).

20 Adsorption of tetrathiafulvalene (TTF) on Cu(100): can pi-stacked 1-D aggregates be formed at low temperature?

Sarasola A, Barja S, de Parga ALV, and Arnau A. Chemical Physics Letters 612, 45 (2014).

21 Applied computational chemistry.

Fernandez I, and Cossio FP. Chemical Society Reviews 43, 4906 (2014).

22 Aromaticity in transition structures.

Schleyer PV, Wu JI, Cossio FP, and Fernandez I. Chemical Society Reviews 43, 4909 (2014).

23 DNA intercalating Ru-II polypyridyl complexes as effective photosensitizers in photodynamic therapy.

Mari C, Pierroz V, Rubbiani R, Patra M, Hess J, Spingler B, Oehninger L, Schur J, Ott I, Salassa L, Ferrari S, and Gasser G. Chemistry-A European Journal 20, 14421 (2014).

24 Distortions of pi-coordinated arenes with anionic character.

Falceto A, Casanova D, Alemany P, and Alvarez S. Chemistry-A European Journal 20, 14674 (2014).

25 Cytotoxic gold(I) N-heterocyclic carbene complexes with phosphane ligands as potent enzyme inhibitors.

Rubbian R, Salassa L, de Almeida A, Casini A, and Ott I. Chemmedchem 9, 1205 (2014).

26 Boron and other triel Lewis acid centers: from hypovalency to hypervalency.

Grabowski SJ. Chemphyschem: a European journal of chemical physics and physical chemistry 15, 2985 (2014).

27 Clusters of ammonium cation-hydrogen Bond versus sigma-hole Bond.

Grabowski SJ. Chemphyschem: a European journal of chemical physics and physical chemistry 15, 876 (2014).

28 Coverage dependence of the level alignment for methanol on TiO₂(110).

Migani A, and Mowbray DJ. Computational and Theoretical Chemistry 1040, 259 (2014).

29 New 'aggregation induced emission (AIE)' active cyclometalated iridium(III) based phosphorescent sensors: high sensitivity for mercury(II) ions.

Alam P, Kaur G, Climent C, Pasha S, Casanova D, Alemany P, Choudhury AR, and Laskar IR. Dalton Transactions 43, 16431 (2014).

30 Contribution of evanescent waves to the effective medium of disordered waveguides.

Yepez M, and Saenz JJ.

EPL 108, 17006 (2014).

31 Structural and electronic properties of magnetic cylinders at the atomic scale.

Aguilera-Granja F, Montejano-Carrizales JM, and Vogel EE.

European Physical Journal D 68, 38 (2014).

32 High pressure phases of different tetraboranes.

Suarez-Alcubilla A, Gurtubay IG, and Bergara A.

High Pressure Research 34, 59 (2014).

33 Stereochemistry of complexes with double and triple metal-ligand bonds: a continuous shape measures analysis.

Alvarez S, Menjon B, Falceto A, Casanova D, and Alemany P.

Inorganic Chemistry 53, 12151, (2014).

34 Application of the level set method for the visual representation of continuous cellular automata oriented to anisotropic wet etching.

Montoliu C, Ferrando N, Cerdá J and Colom RJ.

International Journal of Computer Mathematics 91, 124 (2014).

35 Hole-phonon relaxation and photocatalytic properties of titanium dioxide and zinc oxide: first-principles approach.

Zhukov VP, Tyuterev VG, Chulkov EV, and Echenique PM.

International Journal of Photoenergy 738921 (2014).

36 Perspective on natural orbital functional theory.

Piris M, and Ugalde JM.

International Journal of Quantum Chemistry 114, 1169 (2014).

37 Are there really Cooper pairs and persistent currents in aromatic molecules?

Squire RH, March NH, and Rubio A.

International Journal of Quantum Chemistry 114, 437 (2014).

38 Atomic structure and phonons of a Pb ultrathin film on the Al(100) surface.

Rusina GG, Borisova SD, and Chulkov EV.

Jetp Letters 100, 237 (2014).

39 Dynamics of the BiTeI lattice at high pressures.

Ponosov YS, Kuznetsova TV, Tereshchenko OE, Kokh KA, and Chulkov EV.

Jetp Letters 98, 557 (2014).

40 The phase equilibria in the Ag_2S - Ag_8GeS_6 - Ag_8SnS_6 system.

Aliyeva ZM, Bagheri SM, Aliev ZS, Alverdiyev IJ, Yusibov YA, and Babanly MB.

Journal of Alloys and Compounds 611, 395 (2014).

41 Dielectric spectroscopy at the nanoscale by atomic force microscopy: A simple model linking materials properties and experimental response.

Miccio LA, Kummali MM, Schwartz GA, Alegria A, and Colmenero J.

Journal of Applied Physics 115, 184305 (2014).

42 Local versus global electronic properties of chalcopyrite alloys: X-ray absorption spectroscopy and ab initio calculations.

Sarmiento-Perez R, Botti S, Schnohr CS, Lauermaun I, Rubio A, and Johnson B.

Journal of Applied Physics 116, 093703 (2014).

43 Dielectric spectra broadening as a signature for dipole-matrix interaction. IV. Water in amino acids solutions.

Levy E, Cerveny S, Ermolina I, Puzenko A, and Feldman, Y.

Journal of Chemical Physics 140, 135104 (2014).

44 Second-order perturbative corrections to the restricted active space configuration interaction with the hole and particle approach.

Casanova D.

Journal of Chemical Physics 140, 144111 (2014).

45 The interaction of organic adsorbate vibrations with substrate lattice waves in methyl-Si(111)-(1x1).

Brown RD, Hund ZM, Campi D, O'Leary LE, Lewis NS, Bernasconi M, Benedek G, and Sibener SJ.

Journal of Chemical Physics 141, 024702 (2014).

46 Interacting pairs in natural orbital functional theory.

Piris M.

Journal of Chemical Physics 141, 044107 (2014).

47 Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111).

Kroes GJ, Pavanello M, Blanco-Rey M, Alducin M, and Auerbach DJ.

Journal of Chemical Physics 141, 054705 (2014).

48 Quasi-particle energy spectra in local reduced density matrix functional theory.

Lathiotaki NN, Helbig N, Rubio A, and Gidopoulos NI.

Journal of Chemical Physics 141, 164120 (2014).

49 Two new constraints for the cumulant matrix.

Ramos-Cordoba E, Salvador P, Piris M, and Matito E.

Journal of Chemical Physics 141, 234101 (2014).

50 Vibrational lifetimes of hydrogen on lead films: An ab initio molecular dynamics with electronic friction (AIMDEF) study.

Saalfrank P, Juaristi JI, Alducin M, Blanco-Rey M, and Diez Muino R.

Journal of Chemical Physics 141, 234702 (2014).

51 Nonadiabatic and time-resolved photoelectron spectroscopy for molecular systems.

Flick J, Appel H, and Rubio A.

Journal of Chemical Theory and Computation 10, 1665 (2014).

52 Quasiparticle level alignment for photocatalytic interfaces.

Migani A, Mowbray DJ, Zhao J, Petek H, and Rubio A.

Journal of Chemical Theory and Computation 10, 2103 (2014).

53 **New approximation to the third-order density. Application to the calculation of correlated multicenter indices.**

Feixas F, Sola M, Barroso JM, Ugalde JM, and Matito E.
Journal of Chemical Theory and Computation 10, 3055 (2014).

54 **Electronic structure study of singlet fission in tetracene derivatives.**

Casanova D.
Journal of Chemical Theory and Computation 10, 324 (2014).

55 **Benchmark assessment of density functional methods on group II–VI MX (M = Zn, Cd; X = S, Se, Te) quantum dots.**

Azpiroz JM, Ugalde JM and Infante I.
Journal of Chemical Theory and Computation 10, 76 (2014).

56 **A survey of the parallel performance and accuracy of poisson solvers for electronic structure calculations.**

Garcia-Risueño P, Alberdi-Rodriguez J, Oliveira MJT, Andrade X, Pippig M, Muguerza J, Arruabarrena A, and Rubio A.
Journal of Computational Chemistry 35, 427 (2014).

57 **How much tetraradical character is present in the Si₆ Ge₉ cluster?**

Casanova D.
Journal of computational chemistry 35, 944 (2014).

58 **Electron dynamics of unoccupied states in topological insulators.**

Niesner D, Otto S, Fauster T, Chulkov EV, Ereemeev SV, Tereshchenko OE, and Kokh KA.
Journal of Electron Spectroscopy and Related Phenomena 195, 258 (2014).

59 **Formation of metal-organic interface states studied with 2PPE.**

Marks M, Scholl A, and Hofer U.
Journal of Electron Spectroscopy and Related Phenomena 195, 263 (2014).

60 **Unoccupied electronic structure and relaxation dynamics of Pb/Si(111).**

Sandhofe M, Sklyadneva IY, Sharma V, Trontl VM, Zhou P, Ligges M, Heid R, Bohnen KP, Chulkov EV, and Bovensiepen U.
Journal of Electron Spectroscopy and Related Phenomena 195, 278 (2014).

61 **Whispering gallery mode emission from a composite system of J-aggregates and photonic microcavity.**

Melnikau D, Savateeva D, Rusakov KI, and Rakovich YP.
Journal of Luminescence 145, 138 (2014).

62 **Effect of Tm³⁺ codoping on the near-infrared and upconversion emissions of Er³⁺ in TeO₂-ZnO-ZnF₂ glasses.**

Miguel A, Arriandiaga MA, Morea R, Fernandez J, Gonzalo J, and Balda R.
Journal of Luminescence 154, 136 (2014)

63 **Structural, electronic and magnetic properties of ConPtM-n for M=13, 19, and 55, from first principles.**

Montejano-Carrizales JM, Aguilera-Granja F, Goyhenex C, Pierron-Bohnes V, and Moran-Lopez, JL.
Journal of Magnetism and Magnetic Materials 355, 215 (2014).

64 **Resistive switching dependence on atomic layer deposition parameters in HfO₂-based memory devices.**

Zazpe R, Ungureanu M, Golmar F, Stoliar P, Llopis R, Casanova F, Pickup, DF, Rogero C, and Hueso LE.
Journal of Materials Chemistry C 2, 3204 (2014).

65 **Anisotropic etching on Si{110}: experiment and simulation for the formation of microstructures with convex corners.**

Pal P, Gosalvez MA, Sato K, Hida H, and Xing Y.
Journal of Micromechanics and Microengineering 24, 125001 (2014).

66 **CdS nanoclusters doped with divalent atoms.**

Jimenez-Izal E, Azpiroz JM, Gupta R, Matxain JM, and Ugalde JM.
Journal of Molecular Modeling 20, 2227 (2014).

67 **Spin-orbit effects on the structural, homotop, and magnetic configurations of small pure and Fe-doped Pt clusters.**

Alvarado-Leyva PG, Aguilera-Granja F, García-Fuente A, and Vega A.
Journal of Nanoparticle Research 16, 2222 (2014).

68 **Carbo-cages: a computational study.**

Azpiroz JM, Islas R, Moreno D, Fernandez-Herrera MA, Pan S, Chattaraj PK, Pratim K, Martinez-Guajardo G, Ugalde JM, and Merino G.
Journal of Organic Chemistry 79, 5463 (2014).

69 **Linear and nonlinear optical effects induced by energy transfer from semiconductor nanoparticles to photosynthetic biological systems.**

Rakovich A, Donegan JF, Oleinikov V, Molinari M, Sukhanova A, Nabiev I, and Rakovich YP.
Journal of Photochemistry and Photobiology C-Photochemistry Reviews 20, 17 (2014).

70 **DFT/TDDFT study of the adsorption of N3 and N719 Dyes on ZnO(10 $\bar{1}$ 0) surfaces.**

Azpiroz JM, and De Angelis F.
Journal of Physical Chemistry A 118, 5885 (2014).

71 **Optical properties of 4-bromobenzaldehyde derivatives in chloroform solution.**

Climent C, Alemany P, Lee D, Kim J, and Casanova D.
Journal of Physical Chemistry A 118, 6914 (2014).

72 **Aluminum interaction with glutamate and alpha-Ketoglutarate: a computational study.**

Mujika JI, Ugalde JM, and Lopez X.
Journal of Physical Chemistry B 118, 6680 (2014).

73 **Evolutionary kinetic Monte Carlo: atomistic rates of surface-mediated processes from surface morphologies.**

Ferrando, N, Gosalvez MA, and Ayuela A.
Journal of Physical Chemistry C 118, 11636 (2014).

74 **Antiferromagnetism in Nanofilms of Mn-Doped GaN.**

Echeverria-Arrondo C, Perez-Conde J, and Ayuela A.
Journal of Physical Chemistry C 118, 18064 (2014).

- 75 **Asymmetric response toward molecular fluorination in binary Copper-Phthalocyanine/Pentacene assemblies.**
de Oteyza DG, Garcia-Lastra JM, Goiri E, El-Sayed A, Wakayama Y, and Ortega, JE.
Journal of Physical Chemistry C 118, 18626 (2014).
- 76 **Exploring the surface chemical reactivity of single crystals of binary and ternary bismuth chalcogenides.**
Politano A, Caputo M, Nappini S, Bondino F, Magnano E, Aliev ZS, Babanly MB, Goldoni A, Chiarello G, and Chulkov EV.
Journal of Physical Chemistry C 118, 21517 (2014).
- 77 **Identifying highly conducting Au-C links through inelastic electron tunneling spectroscopy.**
Foti G, Vazquez H, Sanchez-Portal D, Arnau A, and Frederiksen T.
Journal of Physical Chemistry C 118, 27106 (2014).
- 78 **Massive surface reshaping mediated by metal-organic complexes.**
Abadia M, Gonzalez-Moreno R, Sarasola A, Otero-Irurueta G, Verdini A, Floreano L, Garcia-Lekue A, and Rogero C.
Journal of Physical Chemistry C 118, 29704 (2014).
- 79 **Effect of structural dynamics on the opto-electronic properties of bare and hydrated ZnS QDs.**
Azpiroz JM, Mosconi E, Ugalde JM, and De Angelis F.
Journal of Physical Chemistry C 118, 3274 (2014).
- 80 **Quantum dot photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer mechanism driven by electronic coupling.**
Infante I, Azpiroz JM, Blanco NG, Ruggiero E, Ugalde JM, Mareque-Rivas JC, and Salassa L.
Journal of Physical Chemistry C 118, 8712 (2014).
- 81 **Resonant lifetime of core-excited organic adsorbates from first principles.**
Fratesi G, Motta C, Trioni MI, Brivio GP, and Sanchez-Portal D.
Journal of Physical Chemistry C 118, 8775 (2014).
- 82 **Natural orbital functional calculations of molecular polarizabilities and second hyperpolarizabilities. The hydrogen molecule as a test case.**
Lopez X, Piris M, Nakano M, and Champagne B.
Journal of Physics B-atomic Molecular and Optical Physics 47, 015101 (2014).
- 83 **Modelling the effect of nuclear motion on the attosecond time-resolved photoelectron spectra of ethylene.**
Crawford-Uranga A, De Giovannini U, Mowbray DJ, Kurth S, and Rubio A.
Journal of Physics B-Atomic Molecular and Optical Physics 47, 124018 (2014).
- 84 **Circular dichroism in XUV + IR multiphoton ionization of atoms.**
Kazansky AK, Bozhevolnov AV, Sazhina IP, and Kabachnik NM.
Journal of Physics B: Atomic, Molecular and Optical Physics 47, 065602 (2014).
- 85 **The origin of two-dimensional electron gases at oxide interfaces: insights from theory.**
Bristowe NC, Ghosez P, Littlewood PB, and Artacho E.
Journal of Physics-Condensed Matter 26, 143201 (2014).
- 86 **Electron-phonon coupling in quantum-well states of the Pb/Si(111) system.**
Ligges M, Sandhofer M, Sklyadneva I, Heid R, Bohnen KP, Freutel S, Rettig L, Zhou P, Echenique PM, Chulkov EV, and Bovensiepen U.
Journal of Physics-Condensed Matter 26, 352001 (2014).
- 87 **Species fractionation in atomic chains from mechanically stretched alloys.**
da Silva Autreto PA, Galvao DS, and Artacho E.
Journal of Physics-Condensed Matter 26, 435304 (2014).
- 88 **Structural characterization of slightly boron-deficient LiB, LiB_{0.9} and LiB_{0.8}, under pressure.**
Suarez-Alcubilla A, Gurtubay IG, and Bergara A.
Journal of Physics-Condensed Matter 26, 475402 (2014).
- 89 **Use of surface plasmons for manipulation of organic molecule quasiparticles and optical properties.**
Despoja V, and Marusic L.
Journal of Physics-Condensed Matter 26, 485012 (2014).
- 90 **Structural modifications of gold thin films produced by thiol-derivatized single-stranded DNA immobilization.**
Arroyo-Hernandez M, Svec M, Rogero C, Briones C, Martin-Gago JA, and Costa-Kramer JL.
Journal of Physics-Condensed Matter 26, 5, 055010 (2014).
- 91 **Relaxation of highly excited carriers in wide-gap semiconductors.**
Tyuterev VG, Zhukov VP, Echenique PM, and Chulkov EV.
Journal of Physics-Condensed Matter 27, 025801 (2014).
- 92 **Anisotropic plasmon-coupling dimerization of a pair of spherical electron gases.**
Gumbs G, Iurov A, Balassis A, and Huang D.
Journal of Physics-Condensed Matter: an Institute of Physics Journal 26, 135601 (2014).
- 93 **Modelling near-surface bound electron states in a 3D topological insulator: analytical and numerical approaches.**
Men'shov VN, Tugushev VV, Menshchikova V, Ereemeev SV, Echenique PM, and Chulkov EV.
Journal of Physics. Condensed Matter: an Institute of Physics Journal 26, 485003 (2014).
- 94 **Multiple scattering calculations for nonreciprocal planar magnetoplasmonic nanostructures.**
Christofi A, Tserkezis C, and Stefanou N.
Journal of Quantitative Spectroscopy & Radiative Transfer 146, 34 (2014).
- 95 **Differential capacitance of ionic liquid interface with graphite: the story of two double layers.**
Kornyshev AA, Luque NB, and Schmickler, W.
Journal of Solid State Electrochemistry 18, 1345 (2014).
- 96 **Photoinduced C-C reactions on insulators toward photolithography of graphene nanoarchitectures.**
Palma CA, Diller K, Berger R, Welle A, Bjork J, Cabellos JL, Mowbray DJ, Papageorgiou AC, Ivleva NP, Matich S, Margapoti E, Niessner R, Menges B, Reichert J, Feng XL, Rader HJ, Klappenberger F, Rubio A, Mullen K, and Barth JV.
Journal of the American Chemical Society 136, 4651 (2014).

- 97 **Structural, optical, and spectroscopic properties of Er³⁺-doped TeO₂-ZnO-ZnF₂ glass-ceramics.**
Miguel A, Morea R, Arriandiaga MA, Hernandez M, Ferrer FJ, Domingo C, Fernandez-Navarro JM, Gonzalo J, Fernandez J, and Balda R.
Journal of the European Ceramic Society 34, 3959 (2014).
- 98 **The response of a ³He Fermi liquid droplet to vibronic excitation of an embedded glyoxal molecule.**
Benedek G, Hizhnyakov V, and Toennies JP.
Journal Physical Chemistry A 118, 6574 (2014).
- 99 **Time-resolved random laser spectroscopy of inhomogeneously broadened systems.**
Fernandez J, Garcia-Revilla S, Carlos LD, Pecoraro E, Arriandiaga MA, and Balda R.
Laser & Photonics Reviews 8, L32 (2014).
- 100 **Microscopic dynamics in nanocomposites of poly(ethylene oxide) and poly(methyl methacrylate) soft nanoparticles: a quasi-elastic neutron scattering study.**
Bhowmik D, Pomposo JA, Juranyi F, Garcia-Sakai V, Zamponi M, Su Y, Arbe A, and Colmenero J.
Macromolecules 47, 1, 304 (2014).
- 101 **Investigation of a nanocomposite of 75 wt % poly(methyl methacrylate) nanoparticles with 25 wt % poly(ethylene oxide) linear chains: a quasielastic neutron scattering, calorimetric, and WAXS study.**
Bhowmik D, Pomposo JA, Juranyi F, Sakai VG, Zamponi M, Arbe A, and Colmenero J.
Macromolecules 47, 3005 (2014).
- 102 **Branch-point motion in architecturally complex polymers: estimation of hopping parameters from computer simulations and experiments.**
Bacova P, Lentzakis H, Read DJ, Moreno AJ, Vlassopoulos D, and Das Ch.
Macromolecules 47, 3362 (2014).
- 103 **Collective features in polyisobutylene. A study of the static and dynamic structure factor by molecular dynamics simulations.**
Khairy Y, Alvarez F, Arbe A, and Colmenero, J.
Macromolecules 47, 447 (2014).
- 104 **Real-space analysis of branch point motion in architecturally complex polymers.**
Bacová P. and Moreno AJ.
Macromolecules 47, 6955 (2014).
- 105 **Efficient route to compact single-chain nanoparticles: photoactivated synthesis via thiol-yne coupling reaction.**
Pérez-Baena I, Asenjo-Sanz I, Arbe A, Moreno AJ, Lo Verso F, Colmenero J, and Pomposo JA.
Macromolecules 47, 8270 (2014).
- 106 **Intercalation and confinement of poly(ethylene oxide) in porous carbon nanoparticles with controlled morphologies.**
Barroso-Bujans F, Palomino P, Fernandez-Alonso F, Rudic S, Alegria A, Colmenero J, and Enciso E.
Macromolecules 47, 8729 (2014).
- 107 **Assessment of the second-order perturbative corrections to PNOF5.**
Piris M, Ruiperez F, and Matxain JM.
Molecular Physics 112, 1 (2014).
- 108 **Stacking boundaries and transport in bilayer graphene.**
San-Jose P, Gorbachev RV, Geim AK, Novoselov KS, and Guinea F.
Nano Letters 14, 2052 (2014).
- 109 **Complex chiral colloids and surfaces via high-index off-cut silicon.**
McPeak KM, van Engers CD, Blome M, Park JH, Burger S, Gosalvez MA, Faridi A, Ries YR, Sahu A, and Norris, DJ.
Nano Letters 14, 2934 (2014).
- 110 **Co nanodot arrays grown on a GdAu₂ template: substrate/nanodot antiferromagnetic coupling.**
Fernández L, Blanco-Rey M, Ilyn M, Vitali L, Magaña A, Correa A, Ohresser P, Ortega JE, Ayuela A, and Schiller F.
Nano Letters 14, 2977 (2014).
- 111 **Probing the site-dependent kondo response of nanostructured graphene with organic molecules.**
Garnica M, Stradi D, Calleja F, Barja S, Diaz C, Alcamí M, Arnau A, de Parga ALV, Martin F, and Miranda R.
Nano Letters 14, 4560 (2014).
- 112 **Tunable plasmon modes in single silver nanowire optical antennas characterized by far-field microscope polarization spectroscopy.**
Fu M, Qian LH, Long H, Wang K, Lu PX, Rakovich YP, Hetsch F, Susha AS, and Rogach AL.
Nanoscale 6, 9192 (2014).
- 113 **Optical properties and sensing in plexcitonic nanocavities: from simple molecular linkers to molecular aggregate layers.**
Perez-Gonzalez O, Zabala N, and Aizpurua J .
Nanotechnology 25, 035201 (2014).
- 114 **Strong ferromagnetism at the surface of an antiferromagnet caused by buried magnetic moments.**
Chikina A, Hoppner M, Seiro S, Kummer K, Danzenbacher S, Patil S, Generalov A, Guttler M, Kucherenko Y, Chulkov EV, Koroteev YM, Kopernik K, Geibel C, Shi M, Radovic M, Laubschat C, and Vyalikh DV.
Nature Communications 5, 3171 (2014).
- 115 **Determining the polarization state of an extreme ultraviolet free-electron laser beam using atomic circular dichroism.**
Mazza T, Ilchen M, Rafipoor AJ, Callegari C, Finetti P, Plekan O, Prince KC, Richter R, Danailov MB, Demidovich A, De Ninno G, Grazioli C, Ivanov R, Mahne N, Raimondi L, Svetina C, Avaldi L, Bolognesi P, Coreno M, O’Keeffe P, Di Fraia M, Devetta M, Ovchare
Nature Communications 5, 3648 (2014).
- 116 **Chemical control of electrical contact to sp(2) carbon atoms.**
Frederiksen T, Foti G, Scheurer F, Speisser V, and Schull G.
Nature communications 5, 3659 (2014).
- 117 **Graphitic nanostripes in silicon carbide surfaces created by swift heavy ion irradiation.**
Ochedowski O, Osmani O, Schade M, Bussmann BK, Ban-d’Etat B, Lebius H, and Schleberger M.
Nature Communications 5, 3913 (2014).
- 118 **Threading plasmonic nanoparticle strings with light.**
Herrmann LO, Valev VK, Tserkezis C, Barnard JS, Scherman OA, Aizpurua J, and Baumberg JJ.
Nature Communications 5, 4568 (2014).

- 119 **Local determination of the amount of integration of an atom into a crystal surface.**
Volgmann K, Gawronski H, Zaum C, Rusina GG, Borisova SD, Chulkov EV, and Morgenstern K.
Nature Communications 5, 5089 (2014).
- 120 **Strong coupling of single emitters interacting with phononic infrared antennae.**
Esteban R, Aizpurua J, and Bryant GW.
New Journal of Physics 16, 013052 (2014).
- 121 **Magneto-optical Kerr effect in resonant subwavelength nanowire gratings.**
Marinchio H, Carminati R, Garcia-Martin A, and Saenz JJ.
New Journal of Physics 16, 015007 (2014).
- 122 **One-dimensional potential for image-potential states on graphene.**
de Andres PL, Echenique PM, Niesner D, Fauster TH, and Rivacoba A.
New Journal of Physics 16, 023012 (2014).
- 123 **A chemically inert Rashba split interface electronic structure of C_{60} , FeOEP and PTCDA on $BiAg_2/Ag(111)$ substrates.**
Cottin MC, Lobo-Checa J, Schaffert J, Bobisch CA, Moller R, Ortega JE, and Walter AL.
New Journal of Physics 16, 045002 (2014).
- 124 **Helmholtz Fermi surface harmonics: an efficient approach for treating anisotropic problems involving Fermi surface integrals.**
Eiguren A and G. Gurtubay I.
New Journal of Physics 16, 063014 (2014).
- 125 **Quantum ricochets: surface capture, release and energy loss of fast ions hitting a polar surface at grazing incidence.**
Lucas AA, Sunjic M, Benedek G, and Echenique PM.
New Journal of Physics 16, 063015 (2014).
- 126 **The gigantic Rashba effect of surface states energetically buried in the topological insulator Bi_2Te_2Se .**
Miyamoto K, Okuda T, Nurmamat M, Nakatake M, Namatame H, Taniguchi M, Chulkov EV, Kokh KA, Tereshchenko OE, and Kimura A.
New Journal of Physics 16, 065016 (2014).
- 127 **Giant diamagnetism of gold nanorods.**
Hernando A, Ayuela A, Crespo P, and PM Echenique PM.
New Journal of Physics 16, 073043 (2014).
- 128 **Relativistic force between fast electrons and planar targets.**
Rivacoba A, and Zabala N.
New Journal of Physics 16, 073048 (2014).
- 129 **Defect and structural imperfection effects on the electronic properties of BiTeI surfaces.**
Fiedler S, El-Kareh L, Eremeev SV, Tereshchenko OE, Seibel C, Lutz P, Kokh KA, Chulkov EV, Kuznetsova TV, Grebennikov VI, Bentmann H, Bode M, and Reinert F.
New Journal of Physics 16, 075013 (2014).
- 130 **Acoustic plasmons in extrinsic free-standing graphene.**
Pisarra M, Sindona A, Riccardi P, Silkin VM, and Pitarke JM.
New Journal of Physics 16, 083003 (2014).
- 131 **Electronic properties of graphene grain boundaries.**
Ayuela A, Jaskolski W, Santos H, and Chico L.
New Journal of Physics 16, 083018 (2014).
- 132 **Germanene: a novel two-dimensional germanium allotrope akin to graphene and silicene.**
Dávila ME, Xian L, Cahangirov S, Rubio A, and Le Lay G.
New Journal of Physics 16, 095002 (2014).
- 133 **Superspin glass phase and hierarchy of interactions in multiferroic $PbFe_{1/2}Sb_{1/2}O_3$: An analog of ferroelectric relaxors?**
Laguta VV, Stephanovich VA, Savinov M, Marysko M, Kuzian RO, Kondakova IV, Olekhnovich NM, Pushkarev AV, Radyush YV, Raevski IP, Raevskaya SI, and Prosandeev SA.
New Journal of Physics 16, 113041 (2014).
- 134 **Metallic thin films on stepped surfaces: lateral scattering of quantum well states.**
Schiller F, Abd El-Fattah ZM, Schirone S, Lobo-Checa J, Urdanpilleta M, Ruiz-Oses M, Cordon J, Corso M, Sanchez-Portal D, Mugarza A, and Ortega JE.
New Journal of Physics 16, 123025 (2014).
- 135 **Trajectory-dependent energy loss for swift He atoms axially scattered off a silver surface.**
Rubiano CAR, Bocan GA, Juaristi JI, and Gravielle MS.
Nuclear Instruments and Methods in Physics Research Section B-beam Interactions with Materials and Atoms 340, 15 (2014).
- 136 **Effects of pumping wavelength and pump density on the random laser performance of stoichiometric Nd crystal powders.**
Azkargorta J, Iparraguirre I, Bettinelli M, Cavalli E, Barredo-Zuriarrain M, Garcia-Revilla S, Balda R, Fernandez J.
Optics Express 22, 27365 (2014)
- 137 **Optical response of threaded chain plasmons: from capacitive chains to continuous nanorods.**
Tserkezis Ch, Herrmann LO, Valev VK, Baumberg JJ, and Javier Aizpurua J.
Optics Express, 22, 23851 (2014).
- 138 **Molecular dipole, dye structure and electron lifetime relationship in efficient dye sensitized solar cells based on donor-pi-acceptor organic sensitizers.**
Climent C, Cabau L, Casanova D, Wang P, and Palomares E.
Organic Electronics 15, 3162 (2014).
- 139 **Optical response of metallic nanoparticle heteroaggregates with subnanometric gaps.**
Tserkezis Ch, Taylor RW, Beitner J, Esteban R, Baumberg JJ, and Aizpurua J.
Particle & Particle Systems Characterization 31, 152 (2014).
- 140 **Gold spiky nanodumbbells: anisotropy in gold nanostars.**
Novikov SM, Sánchez-Iglesias A, Schmidt MK, Chuvilin A, Aizpurua J, Grzelczak M, and Liz-Marzán LM.
Particle & Particle Systems Characterization 31, 77 (2014).

- 141 **PFO-BPy solubilizers for SWNTs: Modelling of polymers from oligomers.**
Glanzman LN, Mowbray DJ, and Rubio A.
Physica Status Solidi B-Basic Solid State Physics 251, 2407 (2014).
- 142 **Theoretical electron energy loss spectroscopy of isolated graphene.**
Mowbray DJ.
Physica Status Solidi B-Basic Solid State Physics 251, 2509 (2014).
- 143 **Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides.**
Errea I, Calandra M, and Mauri F.
Physica Status Solidi B-Basic Solid State Physics 251, 2556 (2014).
- 144 **Intensity-voltage low-energy electron microscopy for functional materials characterization.**
Flege JI and Krasovskii EE.
Physica Status Solidi-Rapid Research Letters 8, 463 (2014).
- 145 **Tetrel bond– σ -hole bond as a preliminary stage of the S_N2 reaction.**
Grabowski SJ.
Physical Chemistry Chemical Physics 16, 1824 (2014).
- 146 **Mapping the affinity of aluminum(III) for biophosphates: interaction mode and binding affinity in 1:1 complexes.**
Luque NB, Mujika JI, Rezabal E, Ugalde JM, and Lopez X.
Physical Chemistry Chemical Physics 16, 20107 (2014).
- 147 **Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters.**
Aguilera-del-Toro RH, Aguilera-Granja F, Vega A and Balbá LC.
Physical Chemistry Chemical Physics 16, 21732 (2014).
- 148 **Dynamics of supercooled water in a biological model system of the amino acid L-lysine.**
Cervený S, and Swenson J.
Physical Chemistry Chemical Physics 16, 22382 (2014).
- 149 **Topological reaction sites – very strong chalcogen bonds.**
Alikhani ME, Fuster F, Madebène B, and Grabowski SJ.
Physical Chemistry Chemical Physics 16, 2430 (2014).
- 150 **Red-shifting the optical response of firefly oxyluciferin with group 15/16 substitutions.**
Milne, BF.
Physical Chemistry Chemical Physics 16, 24971 (2014).
- 151 **Polymorphic MnAs nanowires of a magnetic shape memory alloy.**
Echeverría-Arrondo C, Perez-Conde J, and Ayuela A.
Physical Chemistry Chemical Physics 16, 5649 (2014).
- 152 **Unveiling mode-selected electron–phonon interactions in metal films by helium atom scattering.**
Benedek G, Bernasconi M, Bohnen KP, Campin D, Chulkov EV, Echenique PM, Heid R, Sklyadneva IYu, and Toennies JP.
Physical Chemistry Chemical Physics 16, 7159 (2014).
- 153 **Polarization control of metal-enhanced fluorescence in hybrid assemblies of photosynthetic complexes and gold nanorods.**
Bujak L, Olejnik M, Brotosudarmo THP, Schmidt MK, Czechowski N, Piatkowski D, Aizpurua J, Cogdell RJ, Heisse W, and Mackowski S.
Physical Chemistry Chemical Physics 16, 9015 (2014).
- 154 **Pulse-delay effects in the angular distribution of near- threshold EUV plus IR two-photon ionization of Ne.**
Mondal S, Fukuzawa H, Motomura K, Tachibana T, Nagaya K, Sakai T, Matsunami K, Yase S, Yao M, Wada S, Hayashita H, Saito N, Callegari C, Prince KC, Miron C, Nagasono M, Togashi T, Yabashi M, Ishikawa KL, Kazansky AK, Kabachnik NM, and Ueda K.
Physical Review A 89, 013415 (2014).
- 155 **Energy-loss contribution to grazing scattering of fast He atoms from a silver surface.**
Rubiano CAR, Bocan GA, Juaristi JI, and Gravielle, MS.
Physical Review A 89, 032706 (2014).
- 156 **Effect of long-range spatial correlations on the lifetime statistics of an emitter in a two-dimensional disordered lattice.**
de Sousa N, Sáenz JJ, García-Martin A, Froufe-Pérez LS, and Marqués MI.
Physical Review A 89, 063830 (2014).
- 157 **Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory.**
Ruggenthaler M, Flick J, Pellegrini C, Appel H, Tokatly IV, and Rubio A.
Physical Review A 90, 012508 (2014).
- 158 **Theoretical study of pulse delay effects in the photoelectron angular distribution of near-threshold EUV plus IR two-photon ionization of atoms.**
Ishikawa KL, Kazansky AK, Kabachnik NM and Ueda K.
Physical Review A 90, 023408 (2014).
- 159 **Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations.**
Lathiotakis NN, Helbig N, Rubio A, and Gidopoulos NI.
Physical Review A 90, 032511 (2014).
- 160 **Attosecond near-threshold photoionization in a strong laser field.**
Kazansky AK, Bozhevolnov AV, Sazhina IP, and Kabachnik NM.
Physical Review A 90, 033409 (2014).
- 161 **Time-dependent density-functional theory of strong-field ionization of atoms by soft x rays.**
Crawford-Uranga A, De Giovannini U, Rasanen E, Oliveira MJT, Mowbray DJ, Nikolopoulos M, Karamatskos ET, Markellos D, Lambropoulos P, Kurth S, and Rubio A.
Physical Review A 90, 033412 (2014).
- 162 **Breakdown of the Peierls substitution for the Haldane model with ultracold atoms.**
Ibanez-Azpiroz J, Eiguren A, Bergara A, Pettini G, and Modugno M.
Physical Review A 90, 033609 (2014).

163 **Optimal control of high-harmonic generation by intense few-cycle pulses.**

Solanpää J, Budagosky JA, Shvetsov-Shilovski NI, Castro A, Rubio A, and Rasanen E.
Physical Review A 90, 053402 (2014).

164 **Probing two-dimensional Anderson localization without statistics.**

Leseur O, Pierrat R, Sáenz JJ, and Carminati R.
Physical Review A 90, 053827 (2014).

165 **Comment on "Weyl fermions and the anomalous Hall effect in metallic ferromagnets".**

Vanderbilt D, Souza I, and Haldane FDM.
Physical Review B (Condensed Matter and Materials Physics) 89, 117101 (2014).

166 **Energy bands in graphene: comparison between the tight-binding model and ab initio calculations.**

Kogan E, Nazarov VU, Silkin VM, and Kaveh M.
Physical Review B (Condensed Matter and Materials Physics) 89, 165430 (2014).

167 **Atomic relaxations at the (0001) surface of Bi₂Se₃ single crystals and ultrathin films.**

Roy S, Meyerheim HL, Mohseni K, Ernst A, Otrokov MM, Vergniory MG, Mussler G, Kampmeier D, Grützmacher D, Tusche C, Schneider J, Chulkov EV, and Kirschner J.
Physical Review B (Condensed Matter and Materials Physics) 90, 155456 (2014).

168 **Effects of 5d electrons and spin-orbit interaction on the characteristics of bulk plasmons in lead.**

Zubizarreta X, Silkin VM, and Chulkov EV.
Physical Review B (Condensed Matter and Materials Physics) 90, 165121 (2014).

170 **Ab initio lattice dynamics and electron-phonon coupling of Bi(111).**

Alcantara Ortigoza M, Sklyadneva IYu, Heid R, Chulkov EV, Rahman TS, Bohnen KP, and chenique PM.
Physical Review B (Condensed Matter and Materials Physics) 90, 195438 (2014).

171 **Magnetism and morphology of Co nanocluster superlattices on GdAu₂/Au(111)-(13×13).**

Cavallin A, Fernande L, Ilyn M, Magana A, Ormaza M, Matena M, Vitali L, Ortega JE, Grazioli C, hresser P, Rusponi S, Brune H, and Schiller F.
Physical Review B (Condensed Matter and Materials Physics) 90, 235419 (2014).

172 **Nontrivial spin structure of graphene on Pt(111) at the Fermi level due to spin-dependent hybridization**

Klimovskikh II, Tsirkin SS, Rybkin AG, Rybkina AA, Filianina MV, Zhizhin EV, and Chulkov EV, and Shikin AM.
Physical Review B (Condensed Matter and Materials Physics) 90, 235431 (2014).

173 **Magnetic interactions in disordered perovskite PbFe_{1/2}Nb_{1/2}O₃ and related compounds: Dominance of nearest-neighbor interaction.**

Kuzian RO, Kondakova IV, Dare AM, and Laguta, VV.
Physical Review B 89, 024402 (2014).

174 **Theory of action spectroscopy for single-molecule reactions induced by vibrational excitations with STM.**

Frederiksen T, Paulsson M, and Ueba H.
Physical Review B 89, 035427 (2014).

175 **Manifestation of a spin-splitting field in a thermally biased Josephson junction.**

Bergeret FS, and Giazotto F.
Physical Review B 89, 054505 (2014).

176 **Magnetic fluctuations in topological insulators with ordered magnetic adatoms: Cr on Bi₂Se₃ from first principles.**

Chotorlishvili L, Ernst A, Dugaev VK, Komnik A, Vergniory MG, Chulkov EV, and Berakdar J.
Physical Review B 89, 075103 (2014).

177 **Bulk and surface electron dynamics in a p-type topological insulator SnSb₂Te₄.**

Niesner D, Otto S, Hermann V, Fauster TH, Menshchikova TV, Ereemeev SV, Aliev ZS, Amiraslanov IR, Babanly MB, Echenique PM, and Chulkov EV.
Physical Review B 89, 081404(R) (2014).

178 **Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation.**

Lu JT, Christensen RB, Foti G, Frederiksen T, Gunst T, and Brandbyge M.
Physical Review B 89, 081405 (2014).

179 **Ab initio analysis of plasmon dispersion in sodium under pressure.**

Ibañez-Azpiroz J, Rousseau B, Eiguren A, and Bergara A.
Physical Review B 89, 085102 (2014).

180 **Many-body interactions and Rashba splitting of the surface state on Cu(110).**

Jiang J, Tsirkin SS, Shimada K, Iwasawa H, Arita M, Anzai H, Namatame H, Taniguchi M, Sklyadneva IYu, Heid R, Bohnen KP, Echenique PM, and Chulkov EV.
Physical Review B 89, 085404 (2014).

181 **Electronic and spin structure of the topological insulator Bi₂Te_{2.4}Se_{0.6}.**

Shikin AM, Klimovskikh II, Ereemeev SV, Rybkina AA, Rusinova MV, Rybkin AG, Zhizhin EV, Sánchez-Barriga J, Varykhalov A, Rusinov IP, Chulkov EV, Kokh KA, Golyashov VA, Kamyshlov V, and Tereshchenko OE.
Physical Review B 89, 125416 (2014).

182 **Spin-orbit coupling as a source of long-range triplet proximity effect in superconductor-ferromagnet hybrid structures.**

Bergeret FS, and Tokatly IV.
Physical Review B 89, 134517 (2014).

183 **Fully self-consistent GW and quasiparticle self-consistent GW for molecules.**

Koval P, Foerster D, and Sanchez-Portal D.
Physical Review B 89, 155417 (2014).

184 **Influence of the surface band structure on electron emission spectra from metal surfaces.**

Archubi CD, Faraggi MN, Silkin VM, and Gravielle MS.
Physical Review B 89, 155421 (2014).

185 **Exchange interaction and its tuning in magnetic binary chalcogenides.**

Vergniory MG, Otrokov MM, Thonig D, Hoffmann M, Maznichenko IV, Geilhufe M, Zubizarreta X, Ostanin S, Marmodoro A, Henk J, Hergert W, Mertig I, Chulkov EV, and Ernst A.
Physical Review B 89, 165202 (2014).

186 **Combined effect of stacking and magnetic field on plasmon excitations in bilayer graphene.**

Wu JY, Gumbs G, and Lin MF.
Physical Review B 89, 165407 (2014).

187 **Role of surface passivation in the formation of Dirac states at polar surfaces of topological crystalline insulators: The case of SnTe(111).**

Eremeev SV, Koroteev YM, Nechaev IA, and Chulkov EV.
Physical Review B 89, 165424 (2014).

188 **Using surface plasmonics to turn on fullerene's dark excitons.**

Despoja V, and Mowbray DJ.
Physical Review B 89, 195433 (2014).

189 **Silicene versus two-dimensional ordered silicide: atomic and electronic structure of Si-($\sqrt{19} \times \sqrt{19}$)R23.4 degrees/Pt(111).**

Svec M, Hapala P, Ondracek M, Merino P, Blanco-Rey M, Mutombo P, Vondracek M, Polyak Y, Chab V, Martin-Gago JA, and Jelinek P.
Physical Review B 89, 201412 (2014).

190 **Plasmaron excitations in p(2 x 2)-K/graphite.**

Chis V, Silkin VM, and Hellsing B.
Physical Review B 89, 205429 (2014).

191 **Revealing Hofstadter spectrum for graphene in a periodic potential.**

Gumbs G, Iurov A, Huang D, and Zhemchuzhna L.
Physical Review B 89, 241407(R) (2014).

192 **Atomic structure of the $\sqrt{3} \times \sqrt{3}$ phase of silicene on Ag(111).**

Cahangirov S, Ozcelik VO, Xian LD, Avila J, Cho S, Asensio MC, Ciraci S, and Rubio A.
Physical Review B 90, 035448 (2014).

193 **Exchange integrals in Mn- and Co-doped II-VI semiconductors.**

Savoyant A, D'Ambrosio S, Kuzian RO, Dare AM, and Stepanov A.
Physical Review B 90, 075205 (2014).

194 **Benchmarking van der Waals functionals with noncontact RPA calculations on graphene-Ag(111).**

Loncaric I, and Despoja V.
Physical Review B 90, 075414 (2014).

195 **Plasmons in a superlattice of fullerenes or metallic shells.**

Balassis A, and Gumbs G.
Physical Review B 90, 075431 (2014).

196 **Spectroscopy and dynamics of unoccupied electronic states of the topological insulators Sb₂Te₃ and Sb₂Te₂S.**

Reimann J, Gudde J, Kuroda K, Chulkov EV, and Hofer U.
Physical Review B 90, 081106 (2014).

197 **First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory.**

Caruso F, Atalla V, Ren XG, Rubio A, Scheffler M, and Rinke P.
Physical Review B 90, 085141 (2014).

198 **Silicite: The layered allotrope of silicon.**

Cahangirov S, Ozcelik VO, Rubio A, and Ciraci S.
Physical Review B 90, 085426 (2014).

199 **Microscopic origin of the relativistic splitting of surface states.**

Krasovskii, EE.
Physical Review B 90, 115434 (2014).

200 **High-energy collective electronic excitations in layered transition-metal dichalcogenides.**

Cudazzo P, Ruotsalainen KO, Sahle CJ, Al-Zein A, Berger H, Navarro-Moratalla E, Huotari S, Gatti M, and Rubio A.
Physical Review B 90, 125125 (2014).

201 **How disorder affects the Berry-phase anomalous Hall conductivity: a reciprocal-space analysis.**

Bianco R, Resta R, and Souza I.
Physical Review B 90, 125153 (2014).

202 **On-surface synthesis of a two-dimensional porous coordination network: Unraveling adsorbate interactions.**

Matena M, Bjork J, Wahl M, Lee TL, Zegenhagen J, Gade LH, Jung TA, Persson M, and Stohr M.
Physical Review B 90, 125408 (2014).

203 **Lieb-Mattis ferrimagnetic superstructure and superparamagnetism in Fe-based double perovskite multiferroics.**

Kuzian RO, Laguta VV, and Richter J.
Physical Review B 90, 134415 (2014)

204 **Ab initio nanoplasmonics: The impact of atomic structure.**

Zhan P, Feist J, Rubio A, Garcia-Gonzalez P, and Garcia-Vidal FJ.
Physical Review B 90, 161407 (2014).

205 **Interplay between structure and electronic properties of layered transition-metal dichalcogenides: comparing the loss function of 1T and 2H polymorphs.**

Cudazzo P, Gatti M, and Rubio A.
Physical Review B 90, 205128 (2014).

206 **Superconducting pairing mediated by spin fluctuations from first principles.**

Essenberger F, Sanna A, Linscheid A, Tandetzky F, Profeta G, Cudazzo P and Gross EKV.
Physical Review B 90, 214504 (2014).

207 **Spin-valley relaxation and quantum transport regimes in two-dimensional transition-metal dichalcogenides.**

Ochoa H, Finocchiaro F, Guinea F, and Fal'ko VI.
Physical Review B 90, 235429 (2014).

208 **Local control of the excitation of surface plasmon polaritons by near-field magneto-optical Kerr effect.**

Vincent R, Marinchio H, Saenz JJ, and Carminati R.
Physical Review B 90, 241412 (2014).

- 209 **Theory of coupled spin-charge transport due to spin-orbit interaction in inhomogeneous two-dimensional electron liquids.**
Shen K, Raimondi R, and Vignale G.
Physical Review B 90, 245302 (2014).
- 210 **Predicted very large thermoelectric effect in ferromagnet-superconductor junctions in the presence of a spin-splitting magnetic field.**
Ozaeta A, Virtanen P, Bergeret FS, and Heikkila TT.
Physical Review Letters 112, 057001 (2014).
- 211 **Spin texture of Bi₂Se₃ thin films in the quantum tunneling limit.**
Landolt G, Schreyeck S, Ereameev SV, Slomski B, Muff S, Osterwalder J, Chulkov EV, Gould C, Karczewski G, Brunner K, Buhmann H, Molenkamp LW, and Dil JH.
Physical Review Letters 112, 057601 (2014).
- 212 **Spin-Dependent Electron Scattering at Graphene Edges on Ni(111).**
Garcia-Lekue A, Balashov T, Olle M, Ceballos G, Arnau A, Gambardella P, Sanchez-Portal D, and Mugarza A.
Physical Review Letters 112, 066802 (2014).
- 213 **Electronic friction dominates hydrogen hot-atom relaxation on Pd(100).**
Blanco-Rey M, Juaristi JI, Díez Muiño R, Busnengo HF, Kroes GJ, and Alducin M.
Physical Review Letters 112, 103203 (2014).
- 214 **Self-assembly of bicomponent molecular monolayers: adsorption height changes and their consequences.**
Goiri E, Matena M, El-Sayed A, Lobo-Checa J, Borghetti P, Rogero C, Detlefs B, Duvernay J, Ortega JE, and de Oteyza DG.
Physical Review Letters 112, 117602 (2014).
- 215 **Role of physisorption states in molecular scattering: a semilocal density-functional theory study on O₂/Ag(111).**
Goikoetxea I, Meyer J, Juaristi JI, Alducin M, and Reuter K.
Physical Review Letters 112, 156101 (2014).
- 216 **Stable single-layer honeycomblike structure of silica.**
Ozcelik VO, Cahangirov S, and Ciraci S.
Physical Review Letters 112, 246803 (2014).
- 217 **Surface strain improves molecular adsorption but hampers dissociation for N₂ on the Fe=W(110) surface.**
Goikoetxea I, Juaristi JI, Díez Muiño R, and Alducin M.
Physical Review Letters 113, 066103 (2014).
- 218 **Quantum spin hall effect in two-dimensional crystals of transition-metal dichalcogenides.**
Cazalilla MA, Ochoa H, and Guinea F.
Physical Review Letters 113, 077201 (2014).
- 219 **Polymer chain dynamics: evidence of nonexponential mode relaxation using thermally stimulated depolarization current techniques.**
Arrese-Igor S, Alegria A, and Colmenero J.
Physical Review Letters 113, 078302 (2014).
- 220 **Correlated electron-nuclear dynamics with conditional wave functions.**
Albareda G, Appel H, Franco I, Abedi A, and Rubio A.
Physical Review Letters 113, 083003 (2014).
- 221 **Tuning the Dirac point position in Bi₂Se₃(0001) via surface carbon doping.**
Roy S, Meyerheim HL, Ernst A, Mohseni K, Tusche C, Vergniory MG, Menshchikova TV, Otrokov MM, Ryabishchenkova AG, Aliev ZS, Babanly MB, Kokh KA, Tereshchenko OE, Chulkov EV, Schneider J, and Kirschner J.
Physical Review Letters 113, 116802 (2014).
- 222 **Anisotropic dispersion and partial localization of acoustic surface plasmons on an atomically stepped surface: Au(788).**
Smerieri M, Vattuone L, Savio L, Langer T, Tegenkamp C, Pfnur H, Silkin VM, and Rocca M.
Physical Review Letters 113, 186804 (2014).
- 223 **Instantaneous band gap collapse in photoexcited monoclinic VO₂ due to photocarrier doping.**
Wegkamp D, Herzog M, Xian L, Gatti M, Cudazzo P, McGahan CL, Marvel RE, Haglund RF, Rubio A, Wolf M, Stahler J.
Physical Review Letters 113, 216401 (2014).
- 224 **How many-body effects modify the van der Waals interaction between graphene sheets.**
Dobson JF, Gould T, and Vignale G.
Physical Review X 4, 021040 (2014).
- 225 **Unconventional phase diagram for six heavy rare earth metals showing melting plus magnetic transitions versus the de Gennes factor.**
Ayuela A, and March NH.
Physics and Chemistry and Chemistry of Liquids 52, 650 (2014).
- 226 **The key role of electron-nuclear potential energy in determining the ground-state energy of inhomogeneous electron liquids in both real and model atoms.**
Amovilli C, and March NH.
Physics and Chemistry of Liquids 52, 576 (2014).
- 227 **Crucial combinations of critical exponents for liquids-vapour and ferromagnetic second-order phase transitions.**
March NH.
Physics and Chemistry of Liquids 52, 697 (2014).
- 228 **Weizsacker inhomogeneity kinetic energy term for the inhomogeneous electron liquid characterising some 30 homonuclear diatomic molecules at equilibrium and insight into Teller's theorem in Thomas-Fermi statistical theory.**
Piris M, and March NH.
Physics and Chemistry of Liquids 52, 804 (2014).
- 229 **Generalisation of Zhang's predictions for the critical exponents of the 3d Ising model if alpha not equal 0.**
March NH.
Physics and Chemistry of Liquids 52, 815 (2014).

230 Inclusion of an applied magnetic field of arbitrary strength in the Ising model.

March NH.

Physics Letters A 378, 2295 (2014).

231 Ab initio calculations of the electron-phonon interaction and characteristics of large polarons in rutile and anatase.

Zhukov VP, and Chulkov EV.

Physics of the Solid State 56, 1302 (2014).

232 Dynamic study of polystyrene-block-poly(4-vinylpyridine) copolymer in bulk and confined in cylindrical nanopores.

Maiz J, Zhao W, Gu Y, Lawrence J, Arbe A, Alegria A, Emrick T, Colmenero J, Russell T, and Mijangos C.

Polymer 55, 4057 (2014).

233 Zwitterionic polymerization of glycidyl monomers to cyclic polyethers with $B(C_6F_5)_3$.

Asenjo-Sanz I, Veloso A, Miranda JI, Pomposo JA, and Barroso-Bujans F.

Polymer Chemistry 5, 6905 (2014).

234 Ultracold Fermi gases with emergent SU(N) symmetry.

Cazalilla MA, and Rey AM.

Reports on Progress in Physics 77, 124401 (2014).

235 Coherent ultrafast charge transfer in an organic photovoltaic blend.

Falke SM, Rozzi CA, Brida D, Maiuri M, Amato M, Sommer E, De Sio A, Rubio A, Cerullo G, Molinari E, and Lienau C.

Science 344, 6187 (2014).

236 A strategy to create spin-split metallic bands on silicon using a dense alloy layer.

Gruznev DV, Dimitry V, Bondarenko LV, Matetskiy AV, Yakovlev AA, Tupchaya AY,

Eremeev SV, Chulkov EV, Chou JP, Wei CM, Lai MY, Wang YL, Zotov AV, and Saranin AA.

Scientific Reports 4, 4742 (2014).

237 Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations.

Raza Z, Errea I, Oganov AR, and Saitta AM.

Scientific Reports 4, 5889 (2014)

238 Spin-helical Dirac states in graphene induced by polar-substrate surfaces with giant spin-orbit interaction: a new platform for spintronics.

Eremeev EV, Nechaev IA, Echenique PM, and Chulkov EV.

Scientific Reports 4, 6900 (2014).

239 Gold nanorods with sub-nanometer separation using cucurbit[n]uril for SERS applications.

Jones ST, Taylor RW, Esteban R, Abo-Hamed EK, Bomans PHH, N, Sommerdijk NAJM, Aizpurua J,

Baumberg JJ and Scherman OA.

Small 10, 4298 (2014).

240 Multi-orthogonal folding of single polymer chains into soft nanoparticles.

Lo Verso F, Pomposo JA, Colmenero J, and Moreno AJ.

Soft Matter 10, 4813 (2014).

241 Single-chain nanoparticles vs. star, hyperbranched and dendrimeric polymers: Effect of the nanoscopic architecture on the flow properties of diluted solutions.

Perez-Baena I, Moreno AJ, Colmenero J, and Pomposo JEA.

Soft Matter 10, 9454 (2014).

242 Coulomb edge effects in graphene nanoribbons.

Jaskolski W, and Ayuela A.

Solid State Communications 196, 1 (2014).

243 Accounting for the thickness dependence of the T-g in supported PS films via the volume holes diffusion model.

Boucher VM, Cangialosi D, Alegria A, and Colmenero J.

Thermochimica Acta 575, 233 (2014).

244 AFM based dielectric spectroscopy: Extended frequency range through excitation of cantilever higher eigenmodes.

Miccio LA, Kummali MM, Schwartz GA, Alegria A, and Colmenero J.

Ultramicroscopy 146, 55 (2014).