

Publications

1 Nanophotoactivity of porphyrin functionalized polycrystalline ZnO films.

Rogero C, Pickup DF, Colchero J, Azaceta E, Tena-Zaera R, and Palacios-Lidon E.
ACS Applied Materials & Interfaces 8, 16783 (2016).

2 Evolution of plasmonic metamolecule modes in the quantum tunneling regime.

Scholl JA, Garcia-Etxarri A, Aguirregabiria G, Esteban R, Narayan TC, Koh AL, Aizpurua J, and Dionne JA.
ACS Nano 10, 1346 (2016).

3 Tunable band alignment with unperturbed carrier mobility of on-surface synthesized organic semiconducting wires.

Basagni A, Vasseur G, Pignedoli CA, Vilas-Varela M, Pena D, Nicolas L, Vitali L, Lobo-Checa J, de Oteyza DG, Sedona F, Casarin M, Ortega JE, and Sarnbi M.
ACS Nano 10, 2644 (2016).

4 Multiple coexisting Dirac surface states in three-dimensional topological insulator PbBi₆Te₁₀.

Papagno M, Ereemeev SV, Fujii J, Aliev ZS, Babanly MB, Mahatha SK, Vobornik I, Mamedov NT, Pacile D, and Chulkov EV.
ACS Nano 10, 3518 (2016).

5 Graphene tunable transparency to tunneling electrons: a direct tool to measure the local coupling.

Gonzalez-Herrero H, Pou P, Lobo-Checa J, Fernandez-Torre D, Craes F, Martinez-Galera AJ, Ugeda MM, Corso M, Ortega JE, Gomez-Rodriguez JM, Perez R, and Brihuega I.
ACS Nano 10, 5131 (2016).

6 Quantum mechanical description of raman scattering from molecules in plasmonic cavities.

Schmidt MK, Esteban R, Gonzalez-Tudela A, Giedke G, and Aizpurua J.
ACS Nano 10, 6291 (2016).

7 **Substrate-independent growth of atomically precise chiral graphene nanoribbons.**
de Oteyza DG, Garcia-Lekue A, Vilas-Varela M, Merino-Diez N, Carbonell-Sanroma E, Corso M, Vasseur G, Rogero C, Guitian E, Pascual JI, Ortega JE, Wakayama Y, and Pena D.
ACS Nano 10, 9000 (2016).

8 **Arrested dimer's diffusion by self-induced back-action optical forces.**
Luis-Hita J, Saenz JJ, and Marqués MI.
ACS Photonics 3, 1286 (2016).

9 **Spatio-temporal modeling of lasing action in core-shell metallic nanoparticles.**
Cuerda J, Garcia-Vidal FJ, Bravo-Abad J.
ACS Photonics 3, 1952 (2016).

10 **Far-and near-field broad-band magneto-optical functionalities using magnetoplasmonic nanorods.**
Armelles G, Cebollada A, Garcia F, Garcia-Martin A, and de Sousa N.
ACS Photonics 3, 2427 (2016).

11 **Anomalous spectral shift of near- and far-field plasmonic resonances in nanogaps.**
Lombardi A, Demetriadou A, Weller L, Andrae P, Benz F, Chikkaraddy R, Aizpurua J, and Baumberg JJ.
ACS Photonics 3, 471 (2016).

12 **Plasmonic response of metallic nanojunctions driven by single atom motion: quantum transport revealed in optics.**
Marchesin F, Koval P, Barbry, Aizpurua J, and Sanchez-Portal D.
ACS Photonics, 3, 269 (2016).

13 **Multiphase biomineralization: enigmatic invasive siliceous diatoms produce crystalline calcite.**
Hermann E, Motylenko M, Sundareshwar PV, Ereskovsky A, Zglobicka I, Noga T, Plocinski T, Tsurkan MV, Wyroba E, Suski S, Bilski H, Wysokowski M, Stoecker H, Makarova A, Vyalikh D, Walter J, Molodtsov SL, Bazhenov V, Petrenko I, Langer E, Richter A, Nieders
Advanced Functional Materials 26, 2503 (2016).

14 **Multi-component organic layers on metal substrates.**
Goiri E, Borghetti P, El-Sayed A, Ortega JE, and de Oteyza DG.
Advanced Materials 28, 1340 (2016).

15 **Supercontinuum generation in naturally occurring glass sponges spicules.**
Ehrlich H, Maldonado M, Parker AR, Kulchin YN, Schilling J, Kohler B, Skrzypczak U, Simon P, Reiswig HM, Tsurkan MV, Brunner E, Voznesenskiy SS, Bezverbny AV, Golik SS, Nagorny IG, Vyalikh DV, Makarova AA, Molodtsov SL, Kummer K, Mertig M, Erler C, Kurek D
Advanced Optical Materials 4, 1608 (2016).

16 **Growth of Co nanomagnet arrays with enhanced magnetic anisotropy.**
Fernandez L, Ilyn M, Magana A, Vitali L, Ortega JE, and Schiller F.
Advanced Science 3, 1600187 (2016).

17 **Donor-stabilized 1,3-disila-2,4-diazacyclobutadiene with a Nonbonded Si...Si distance compressed to a Si=Si double bond length.**
Gau D, Nogue R, Saffon-Merceron N, Baceiredo A, De Clzar A, Cossio FP, Hashizume D, and Kato T.
Angewandte Chemie International Edition 55, 14673 (2016).

18 **Alkenyl arenes as dipolarophiles in catalytic asymmetric 1,3-dipolar cycloaddition reactions of azomethine ylides.**
Pascual-Escudero A, de Cozar A, Cossio FP, Adrio J, and Carretero JC.
Angewandte Chemie International Edition 55, 15334 (2016).

19 **Peculiar all-metal sigma-aromaticity of the [Au2Sb16](4-) anion in the solid state.**
Popov IA, Pan FX, You XR, Li LJ, Matito E, Liu C, Zhai HJ, Sun ZM, and Boldyrev AI.
Angewandte Chemie International Edition 55, 15344 (2016).

20 **All-metal antiaromaticity in Sb4-type lanthanocene anions.**
Min X, Popov IA, Pan FX, Li LJ, Matito E, Sun ZM, Wang LS, and Alexander I, and Boldyrev AI.
Angewandte Chemie International Edition 55, 5531 (2016).

21 **On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: intrinsic effects revealed by theory and experiment.**
Milne BF, Kjaer C, Houmoller J, Stockett MH, Toker Y, Rubio A, and Nielsen SB.
Angewandte Chemie International Edition 55, 6248 (2016).

22 **[3,3]-sigmatropic rearrangement/allylboration/cyclization sequence: enantioenriched seven-membered-ring carbamates and ring contraction top pyrrolidines.**
Mace A, Touchet S, Andres P, Cossio F, Dorcet V, Carreaux F, and Carboni B.
Angewandte Chemie-International Edition 55, 1025 (2016).

23 **Unusually short be-be distances with and without a Bond in Be2F2 and in the molecular discuses Be2B8 and Be2B7-.**
Cui ZH, Yang WS, Zhao LL, Ding YH, and Frenking G.
Angewandte Chemie-International Edition 55, 7841 (2016).

24 **Modelling graphene quantum dot functionalization via ethylene-dinitrobenzoyl.**
Noori K, Hubener H, Kymakis E, and Giustino F.
Applied Physics Letters 108, 123902 (2016).

25 **Fluence dependent electrical conductivity in aluminium thin films grown by infrared pulsed laser deposition.**
Rebollar E, Martínez-Tong DE, Sanz M, Oujja M, Marco JF, Ezquerra TA, and Castillejo M.
Applied Surface Science 387, 1188 (2016).

26 **MorphoLibJ: integrated library and plugins for mathematical morphology with ImageJ.**
Legland D, Arganda-Carreras I, and Andrey P.
Bioinformatics 32, 3532 (2016).

27 **The electron-pair density distribution of the (1,3)Pi(u) excited states of H-2.**

Mercero JM, Rodriguez-Mayorga M, Matito E, Lopez X, and Ugalde JM.
Canadian Journal of Chemistry 94, 998 (2016).

28 **Absorbate-induced ordering and bilayer formation in propanol-graphite-oxide intercalates.**

Cabrillo C, Barroso-Bujans F, Fernandez-Perea R, Fernandez-Alonso F, Bowron D, and Bermejo FJ.
Carbon 100, 546 (2016).

29 **A Zn based coordination polymer exhibiting long-lasting phosphorescence.**

Cepeda J, Sebastian ES, Padro D, Rodriguez-Dieguez A, Garcia JA, Ugalde JM, Seco JM.
Chemical Communications 52, 8671 (2016).

30 **A push-pull organic dye with a quinoidal thiophene linker:**

Photophysical properties and solvent effects.

Climent C, Carreras A, Alemany P, and Casanova D.
Chemical Physics Letters 663, 45 (2016).

31 **Confined water as model of supercooled water.**

Cervený S, Mallamace F, Swenson J, Vogel M, and Xu LM.
Chemical Reviews 116, 7608 (2016).

32 **Tuning Surface Chemistry of TiC Electrodes for lithium-air batteries.**

Kozmenkova AY, Kataev EY, Belova AI, Arnati M, Gregoratti L, Velasco-Velez J, Knop-Gericke A, Senkovsky B, Vyalikh DV, Itkis DM, Shao-Horn Y, and Yashina LV.
Chemistry of Materials 28, 8248 (2016).

33 **Comparison of hydrogen and gold bonding in [XH_X]⁽⁻⁾, [XAuX]⁽⁻⁾, and isoelectronic [NgHN_g]⁽⁺⁾, [NgAuN_g]⁽⁺⁾ (X=halogen, Ng=noble gas).**

Grabowski SJ, Ugalde JM, Andrada DM, and Frenking G.
Chemistry-A European Journal 22, 11317 (2016).

34 **Reaction mechanism of the hydrogermylation/hydrostannylation of unactivated alkenes with two-coordinate E(II) hydrides (E=Ge, Sn): a theoretical study.**

Zhao L, Hermann M, Jones C, Frenking G.
Chemistry-A European Journal 22, 11728 (2016).

35 **Upconverting nanoparticles prompt remote near-infrared photoactivation of Ru(II)-Arene complexes.**

Ruggiero E, Garino C, Mareque-Rivas JC, Habtemariam A, and Salassa L.
Chemistry-A European Journal 22, 2801 (2016).

36 **The Bond order of C-2 from a strictly N-representable natural orbital energy functional perspective.**

Piris M, Lopez X, and Ugalde, JM.
Chemistry-A European Journal 22, 4109 (2016).

37 **New insights into the reactivity of cisplatin with free and restrained nucleophiles: microsolvation effects and base selectivity in cisplatin-DNA interactions.**

de Cozar A, Larranaga O, Bickelhaupt FM, Sebastian ES, Ortega-Carrasco E, Marechal JD, Lledos A, and Cossio FP.
ChemPhysChem 17, 3932 (2016).

38 **Exploring the origin of "aggregation induced emission" activity and "crystallization induced emission" in organometallic iridium(III) cationic complexes: influence of counterions.**

Alam P, Climent C, Kaur G, Casanova, D, Choudhury AR, Gupta A, Alemany P, and Laskar IR.
Crystal Growth & Design 16, 5738 (2016).

39 **[FHF]⁽⁻⁾ - The strongest hydrogen Bond under the influence of external interactions.**

Grabowski SJ.
Crystals 6, 3 (2016).

40 **Analysis of hydrogen bonds in crystals.**

Grabowski SJ.
Crystals 6, 59 (2016).

41 **Upconverting nanoparticles for the near infrared photoactivation of transition metal complexes: new opportunities and challenges in medicinal inorganic photochemistry.**

Ruggiero E, Alonso-de Castro S, Habtemariam A, and Salassa L.
Dalton Transactions 45, 13012 (2016).

42 **Nanophononics: state of the art and perspectives.**

Volz S, Ordonez-Miranda J, Shchepetov A, Prunnila M, Ahopelto J, Pezeril T, Vaudel G, Gusev V, Ruello P, Weig EM, Schubert M, Hettich M, Grossman M, Dekorsy T, Alzina F, Graczykowski B, Chavez-Angel E, Reparaz JS, Wagner MR, Sotomayor-Torres CM, Xiong SY,
European Physical Journal B 89, 15 (2016).

43 **Thermal smearing and screening in a strong magnetic field for Dirac materials in comparison with the two dimensional electron liquid.**

Gumbs G, Balassis A, Dahal D, and Glasser ML.
European Physical Journal B 89, 234 (2016).

44 **Approaching the strongly anharmonic limit with ab initio calculations of materials' vibrational properties - a colloquium.**

Errea I.
European Physical Journal B 89, 237 (2016).

45 **Anomalous Hall and spin Hall conductivities in three-dimensional ferromagnetic topological insulator/normal insulator heterostructures.**

Men'shov VN, Tugushev VV, and Chulkov EV.
Europhysics Letters 114, 37003 (2016).

46 **Andreev spectrum of a Josephson junction with spin-split superconductors.**

Bujnowski B, Bercioux D, Kanschelle F, Cayssol J, and Bergeret FS.
Europhysics Letters 115, 67001 (2016).

- 47 **Special issue on trends in nanotechnology (TNT2015).**
Correia A, Saenz JJ, and Serena PA,
International Journal of Nanotechnology 13, 571 (2016).
- 48 **Chemical and ionization potentials: relation via the Pauli potential and NOF theory.**
Piris M, and March NH.
International Journal of Quantum Chemistry 116, 805 (2016).
- 49 **Is spillover relevant for hydrogen adsorption and storage in porous carbons doped with palladium nanoparticles?**
Blanco-Rey M, Juaristi JI, Alducin M, López MJ, and AlonsoJA.
Journal of Physical Chemistry C 120, 17357 (2016).
- 50 **Anisotropic electronic, mechanical, and optical properties of monolayer WTe₂.**
Torun E, Sahin H, Cahangirov S, Rubio A, and Peeters FM.
Journal of Applied Physics 119, 074307 (2016).
- 51 **Electron-phonon relaxation and excited electron distribution in gallium nitride.**
Zhukov VP, Tyuterev VG, Chulkov EV, and Echenique PM.
Journal of Applied Physics 120, 085708 (2016).
- 52 **Quantifying local exciton, charge resonance, and multiexciton character in correlated wave functions of multichromophoric systems.**
Casanova D, and Krylov AI.
Journal of Chemical Physics 144, 014102 (2016).
- 53 **Structural and optical properties of the naked and passivated Al₅Au₅ bimetallic nanoclusters.**
Grande-Aztatzi R, Formoso E, Mercero JM, Matxain JM, Grabowski SJ, and Ugalde JM.
Journal of Chemical Physics 144, 114302 (2016).
- 54 **Structure and component dynamics in binary mixtures of poly (2- (dimethylamino) ethyl methacrylate) with water and tetrahydrofuran: a diffraction, calorimetric, and dielectric spectroscopy study.**
Goracci G, Arbe A, Alegría A, Su Y, Gasser U, and Colmenero J.
Journal of Chemical Physics 144, 154903 (2016).
- 55 **Molecular electric moments calculated by using natural orbital functional theory.**
Mitxelena I, and Piris M.
Journal of Chemical Physics 144, 204108 (2016).
- 56 **New structural and electronic properties of (TiO₂)(10).**
Aguilera-Granja F, Vega A, and Balbas LC.
Journal of Chemical Physics 144, 234312 (2016).
- 57 **Modeling surface motion effects in N₂ dissociation on W(110): Ab initio molecular dynamics calculations and generalized Langevin oscillator model.**
Nattino F, Galparsoro O, Costanzo F, Díez Muiño R, Alducin M, and Kroes GJ.
Journal of Chemical Physics 144, 244708 (2016).
- 58 **Electron-hole pair effects in methane dissociative chemisorption on Ni(111).**
Luo X, Jiang B, Juaristi JI, Alducin M, and Guo H.
Journal of Chemical Physics 145, 044704 (2016).
- 59 **Probing the electronic structure and Au-C chemical bonding in AuC_n⁻ and AuC_nH⁻ (n=2, 4, and 6) using high-resolution photoelectron spectroscopy.**
Leon I, Ruiperez F, Ugalde JM, and Wang LS.
Journal of Chemical Physics 145, 064304 (2016).
- 60 **On the tautomerisation of porphycene on copper (111): Finding the subtle balance between van der Waals interactions and hybridisation.**
Novko D, Tremblay JC, and Blanco-Rey M.
Journal of Chemical Physics 145, 244701 (2016).
- 61 **Quantum-classical nonadiabatic dynamics: coupled- vs independent-trajectory methods.**
Agostini F, Min SK, Abedi A, and Gross EKV.
Journal of Chemical Theory and Computation 12, 2127 (2016).
- 62 **Low-lying pi pi* states of heteroaromatic molecules: a challenge for excited state methods.**
Prijs A, Sandoval-Salinas ME, Casanova D, Jacquemin D, and Corninboeuf C.
Journal of Chemical Theory and Computation 12, 2652 (2016).
- 63 **Optical absorption spectra and excitons of dye-substrate interfaces: catechol on TiO₂(110).**
Mowbray DJ, and Migani A.
Journal of Chemical Theory and Computation 12, 2843 (2016).
- 64 **Toward Hamiltonian adaptive QM/MM: accurate solvent structures using many-body potentials.**
Boereboom JM, Potestio R, Donadio D, and Buló RE.
Journal of Chemical Theory and Computation 12, 3441 (2016).
- 65 **Diffusion Monte Carlo perspective on the spin-state energetics of [Fe(NCH)₆](2⁻).**
Fumanal M, Wagner LK, Sanvito S, and Droghetti A.
Journal of Chemical Theory and Computation 12, 4233 (2016).
- 66 **Interplay between aromaticity and strain in double group transfer reactions to 1,2-benzynes.**
Fernandez I, and Cossio FP.
Journal of Computational Chemistry 37, 1265 (2016).
- 67 **The barrier to the methyl rotation in Cis-2-butene and its isomerization energy to trans-2-butene, revisited.**
Matta CF, Sadjadi S, Braden DA, and Frenking G.
Journal of Computational Chemistry 37, 143 (2016).
- 68 **Coherence characteristics of random lasing in a dye doped hybrid powder.**
García-Revilla S, Fernández J, Barredo-Zuriarrain M, Pecoraro E, Arriandiaga MA, Iparraguirre I, Azkargorta J, and Balda R.
Journal of Luminescence 169, 472 (2016).

69 Polarization-selective enhancement of Nd³⁺ photoluminescence assisted by linear chains of silver nanoparticles.

Yraola E, Sanchez-Garcia L, Tserkezis C, Molina P, Ramirez MO, Aizpurua J, and Bausa LE. Journal of Luminescence 169, 569 (2016).

70 Er³⁺-doped fluorotellurite thin film glasses with improved Er³⁺ photoluminescence emission at 1.53 μ m.

Morea R, Miguel A, Fernandez TT, Mate B, Ferrer FJ, Maffiotte C, Fernandez J, Balda R, and Gonzalo J. Journal of Luminescence 170 778 (2016).

71 Transient mechanochromism in epoxy vitrimer composites containing aromatic disulfide crosslinks.

de Luzuriaga AR, Matxain JM, Ruiperez F, Martin R, Asua JM, Cabanero G, and Odriozola I. Journal of Materials Chemistry C 4, 6220 (2016).

72 Fluctuations during anisotropic etching: local recalibration and application to Si{110}.

Gosalvez MA, Li Y, Ferrando N, Pal P, Sato K, and Xing Y. Journal of Microelectromechanical Systems 25, 788 (2016).

73 Evidence for faster etching at the mask-substrate interface: atomistic simulation of complex cavities at the micron-/submicron-scale by the continuous cellular automaton.

Gosalvez MA, Ferrando N, Fedoryshyn Y, Leuthold J, and McPeak KM. Journal of Micromechanics and Microengineering 26, 045013 (2016).

74 Angular distribution and circular dichroism in the two-colour XUV plus NIR above-threshold ionization of helium.

Mazza T, Ilchen M, Rafipoor AJ, Callegari C, Finetti P, Plekan O, Prince KC, Richter R, Demidovich A, Grazioli C, Avaldi L, Bolognesi P, Coreno M, O'Keeffe P, Di Fraia M, Devetta M, Ovcharenko Y, Lyamayev V, Dusterer S, Ueda K, Costello JT, Gryzlova EV, Strakhova SI, Grum-Grzhimailo AN, Bozhevolnov AV, Kazansky AK, Kabachnik NM, and Meyer M. Journal of Modern Optics 63, 367 (2016).

75 Structural, electronic, and magnetic properties of Fe (x) Co (y) Pd (z) (x plus y plus z accuracy sign 7) clusters: a density functional theory study.

Varas A, Aguilera-Granja F, Rogan J, and Kiwi M. Journal of Nanoparticle Research 18, 252 (2016).

76 Stereospecific synthesis of alpha-amino allylsilane derivatives through a [3,3]-allyl cyanate rearrangement. mild formation of functionalized disiloxanes.

Henrion S, Carboni B, Cossio FP, Roisnel T, Villalgorido JM, and Carreaux F. Journal of Organic Chemistry 81, 4633 (2016).

77 4th international conference on chemical bonding.

Ugalde JM, Bultinck P, Bickelhaupt FM, and Alexandrova AN. Journal of Physical Chemistry A 120, 9353 (2016).

78 Optimizing SERS from gold nanoparticle clusters: addressing the near field by an embedded chain plasmon model.

Taylor RW, Esteban R, Mahajan S, Aizpurua J, and Baumberg JJ. Journal of Physical Chemistry C 120, 10512 (2016).

79 Exploring the optical nonlinearities of plasmon-exciton hybrid resonances in coupled colloidal nanostructures.

Simon T, Melnikau D, Sanchez-Iglesias A, Grzelczak M, Liz-Marzan LM, Rakovich Y, Feldmann J, and Urban AS. Journal of Physical Chemistry C 120, 12226 (2016).

80 Electronic structure of low-dimensional carbon pi-systems.

Garcia-Lastra JM, Boukahil I, Qiao RM, Rubio A, and Himpsel FJ. Journal of Physical Chemistry C 120, 12362 (2016).

81 Plasmonic resonances in the Al-13(-) cluster: quantification and origin of exciton collectivity.

Casanova D, Matxain JM, and Ugalde JM. Journal of Physical Chemistry C 120, 12742 (2016).

82 Disentangling vacancy oxidation on metallicity-sorted carbon nanotubes.

Mowbray DJ, Paz AP, Ruiz-Soria G, Sauer M, Lacovig P, Dalmiglio M, Lizzit S, Yanagi K, Goldoni A, Pichler T, Ayala P, and Rubio A. Journal of Physical Chemistry C 120, 18316 (2016).

83 CO₂ binding and induced structural collapse of a surface-supported metal-organic network.

Cechal J, Kley CS, Petuya R, Schramm F, Ruben M, Stepanow S, Arnau A, and Kern K. Journal of Physical Chemistry C 120, 18622 (2016).

84 Intra- and intermolecular singlet fission in covalently linked dimers.

Feng XT, Casanova D, and Krylov AI. Journal of Physical Chemistry C 120, 19070 (2016).

85 Photoinduced absorption within single-walled carbon nanotube systems.

Glanzmann LN, Mowbray DJ, del Valle DGF, Scotognella F, Lanzani G, and Rubio A. Journal of Physical Chemistry C 120, 1926 (2016).

86 Structural, vibrational, and electronic study of alpha-As₂Te₃ under compression.

Cuenca-Gotor VP, Sans JA, Ibanez J, Popescu C, Gomis O, Vilaplana R, Manjon FJ, Leonardo A, Sagasta E, Suarez-Alcubilla A, Gurtubay IG, Mollar M, and Bergara A. Journal of Physical Chemistry C 120, 19340 (2016).

87 Search for a metallic dangling-bond wire on n-doped H-passivated semiconductor surfaces.

Engelund M, Papior N, Brandimarte P, Frederiksen T, Garcia-Lekue A, and Sanchez-Portal D. Journal of Physical Chemistry C 120, 20303 (2016).

88 Metallic and magnetic 2D materials containing planar tetracoordinated C and N.

Jimenez-Izal E, Saeys M, and Alexandrova AN. Journal of Physical Chemistry C 120, 21685 (2016).

89 **Surface Dynamics of the Wetting layers and ultrathin films on a Dynamic Substrate: (0.5-4) ML Pb/Cu(111).**

Rusina GG, Borisova SD, Ereemeev SV, Sklyadneva IY, Chulkov EV, Benedek G, and Toennies JP. *Journal of Physical Chemistry C* 120, 22304 (2016).

90 **Molecular-level realignment in donor-acceptor bilayer blends on metals.**

Borghetti P, de Oteyza DG, Rogero C, Goiri E, Verdini A, Cossaro A, Floreano L, and Ortega JE. *Journal of Physical Chemistry C* 120, 5997 (2016).

91 **Theoretical insight into the internal quantum efficiencies of polymer/C-60 and polymer/SWNT photovoltaic devices.**

Glanzmann LN, and Mowbray DJ. *Journal of Physical Chemistry C* 120, 6336 (2016).

92 **Electron-phonon coupling strength at metal surfaces directly determined from the helium atom scattering debye-waller factor.**

Manson JR, Benedek G, and Miret-Artés. *Journal of Physical Chemistry Letters* 7, 1016 (2016).

93 **AFM imaging of mercaptobenzoic acid on Au(110): submolecular contrast with metal tips.**

Hauptmann N, Robles R, Abufager P, Lorente N, Berndt R. *Journal of Physical Chemistry Letters* 7, 1984 (2016).

94 **Single-molecule conductance through hydrogen bonds: the role of resonances.**

Wimmer M, Palma J, Tarakeshwar P, and Mujica V. *Journal of Physical Chemistry Letters* 7, 2977 (2016).

95 **Electron-hole pair effects in polyatomic dissociative chemisorption: water on Ni(111).**

Jiang B, Alducin M, and Guo H. *Journal of Physical Chemistry Letters* 7, 327 (2016).

96 **Rabi splitting in photoluminescence spectra of hybrid systems of gold nanorods and J-aggregates.**

Melnikau D, Esteban R, Savateeva D, Sanchez-Iglesias AS, Grzelczak M, Schmidt MK, Liz-Marzan LM, Aizpurua J, and Rakovich YP. *Journal of Physical Chemistry Letters* 7, 354 (2016).

97 **Evidence of coupling between the motions of water and peptides.**

Cervený S, Combarro-Palacios I, and Swenson J. *Journal of Physical Chemistry Letters* 7, 4093 (2016).

98 **Concentrated solutions of single-chain nanoparticles: a simple model for intrinsically disordered proteins under crowding conditions.**

Moreno AJ, Lo Verso F, Arbe A, Pomposo JA, and Colmenero J. *Journal of Physical Chemistry Letters* 7, 838 (2016).

99 **Decacyclene trianhydride at functional interfaces: an ideal electron acceptor material for organic electronics.**

de Oteyza DG, Garcia-Lastra JM, Toma FM, Borghetti P, Foreano L, Verdini A, Cossaro A, Pho TV, Wudl F, and Ortega JE. *Journal of Physical Chemistry Letters* 7, 90 (2016).

100 **Angle resolved photoelectron spectroscopy of two-color XUV-NIR ionization with polarization control.**

Dusterer S, Hartmann G, Babies F, Beckmann A, Brenner G, Buck J, Costello J, Dammann L, De Fanis A, Gessler P, Glaser L, Ilchen M, Johnsson P, Kazansky AK, Kelly TJ, Mazza T, Meyer M, Nosik VL, Sazhina IP, Scholz F, Seltmann J, Sotoudi H, Viefhaus J, and K. *Journal of Physics B-Atomic Molecular and Optical Physics* 49, 165003 (2016).

101 **Self-diffusion and structural properties of confined fluids in dynamic coexistence.**

de Sousa N, Saenz JJ, Scheffold F, Garcia-Martin A, and Froufe-Perez LS. *Journal of Physics Condensed Matter* 28, 135101 (2016).

102 **On the stability of the electronic system in transition metal dichalcogenides.**

Faraggi MN, Zubizarreta X, Arnau A, and Silkin VM. *Journal of Physics Condensed Matter* 28, 184004 (2016).

103 **Optical response of silver clusters and their hollow shells from linear-response TDDFT.**

Koval P, Marchesin F, Foerster D, and Sanchez-Portal D. *Journal of Physics Condensed Matter* 28, 214001 (2016).

104 **Electronic and magnetic properties of superconducting LnO(1-x)F(x)BiS(2) (Ln = La, Ce, Pr, and Nd) from first principles.**

Morice C, Artacho E, Dutton SE, Kim HJ, and Saxena SS. *Journal of Physics Condensed Matter* 28, 345504 (2016).

105 **Anharmonic enhancement of superconductivity in metallic molecular Cmca-4 hydrogen at high pressure: a first-principles study.**

Borinaga M, Riego P, Leonardo A, Calandra M, Mauri F, Bergara A, and Errea I. *Journal of Physics Condensed Matter* 28, 494001 (2016).

106 **Plasmon excitations for encapsulated graphene.**

Gumbs G, Horing NJM, Iurov A, and Dahal D. *Journal of Physics D-Applied Physics* 49, 225101 (2016).

107 **Spin-polarised edge states in atomic Mn chains supported on Cu₂N/Cu (100).**

Choi DJ, Robles R, Gauyacq JP, Rubio-Verdu C, Lorente N, and Pascual JI. *Journal of Physics-Condensed Matter* 28, 23LT01 (2016).

108 **Insight on a novel layered semiconductors: CuTlS and CuTlSe.**

Aliev ZS, Zuniga FJ, Koroteev YM, Brezczewski T, Babanly NB, Amiraslanov IR, Politano A, Madariaga G, Babanly MB, and Chulkov EV. *Journal of Solid State Chemistry* 242, 1 (2016).

109 Fully fused quinoidal/aromatic carbazole macrocycles with poly-radical characters.

Das S, Herrng TS, Zafra JL, Burrezo PM, Kitano M, Ishida MY, Gopalakrishna TY, Hu P, Osuka A, Casado J, Ding J, Casanova D, and Wu JS. Journal of the American Chemical Society 138, 7782 (2016).

110 Higher order pi-conjugated polycyclic hydrocarbons with open-shell singlet ground state: nonazethrene versus nonacene.

Huang R, Phan H, Herrng TS, Hu P, Zeng WD, Dong SQ, Das S, Shen YJ, Ding J, Casanova D, and Wu JS. Journal of the American Chemical Society 138, 10323 (2016).

111 Noncovalent dimerization after enediyne cyclization on Au(111).

de Oteyza DG, Paz AP, Chen YC, Pedramrazi Z, Riss A, Wickenburg S, Tsai HZ, Fischer FR, Crommie MF, and Rubio A. Journal of the American Chemical Society 138, 10963 (2016).

112 Mechanistic picture and kinetic analysis of surface-confined Ullmann polymerization.

Di Giovannantonio M, Tomellini M, Lipton-Duffin J, Galeotti G, Elrahimi M, Cossaro A, Verdini A, Kharche N, Meunier V, Vasseur G, Fagot-Revurat Y, Perepichka DF, Rosei F, and Contini G. Journal of the American Chemical Society 138, 16696 (2016).

113 Gold as a 6p-element in dense lithium aurides.

Yang GC, Wang YC, Peng F, Bergara A, and Ma YM. Journal of the American Chemical Society 138, 4046 (2016).

114 Pi band dispersion along conjugated organic nanowires synthesized on a metal oxide semiconductor.

Vasseur G, Abadia M, Miccio LA, Brede J, Garcia-Lekue A, de Oteyza DG, Rogero C, Lobo-Checa J, and Ortega JE. Journal of the American Chemical Society 138, 5685 (2016).

115 Surface cis effect: influence of an axial ligand on molecular self assembly.

Knaak T, Gopakumar TG, Schwager B, Tuzcek F, Robles R, Lorente N, and Berndt R. Journal of the American Chemical Society 138, 7544 (2016).

116 Hybrid cluster-expansion and density-functional-theory approach for optical absorption in TiO₂.

Vanska O, Ljungberg MP, Springer P, Sanchez-Portal D, Kira M, and Koch SW. Journal of the Optical Society of America B Optical Physics 33, C123 (2016).

117 Plasmon response and electron dynamics in charged metallic nanoparticles.

Herrera MZ, Aizpurua J, Kazansky AK, and Borisov AG. Langmuir 32, 2829 (2016).

118 Cholesterol-ceramide interactions in phospholipid and sphingolipid bilayers as observed by positron annihilation lifetime spectroscopy and molecular dynamics simulations.

Garcia-Arribas AB, Axpe E, Mujika JI, Merida D, Busto JV, Sot J, Alonso A, Lopez X, Garcia JA, Ugalde JM, Plazaola, F, and Goñi FM. Langmuir 32, 5434 (2016).

119 New double-infiltration methodology to prepare PCL-PS core-shell nanocylinders inside anodic aluminum oxide templates.

Sanz B, Blaszczyk-Lezak I, Mijangos C, Palacios JK, and Muller AJ. Langmuir 32, 7860 (2016).

120 Random laser action in stoichiometric Nd₃Ga₅O₁₂ garnet crystal powder.

Iparraguirre I, Azkargorta J, Kamada K, Yoshikawa A, Rodriguez-Mendoza UR, Lavin V, Barredo-Zuriarrain M, Balda R, and Fernandez J. Laser Physics Letters 13, 035402 (2016).

121 Antenna-assisted picosecond control of nanoscale phase transition in vanadium dioxide.

Muskens OL, Bergamini L, Wang YD, Gaskell JM, Zabala N, de Groot CH, Sheel DW, and Aizpurua J. Light Science & Applications 5, e16173 (2016).

122 Structural exploration of phantom oligoguanidine from asymmetric diamine and guanidine hydrochloride.

Wang H, Bethke C, Hermann M, Frenking G, and Agarwal S. Macromolecular Chemistry and Physics 217, 1834 (2016).

123 A solvent-based strategy for tuning the internal structure of metallo-folded single-chain nanoparticles.

Basasoro S, Gonzalez-Burgos M, Moreno AJ, Lo Verso F, Arbe A, Colmenero J, and Pomposo JA. Macromolecular Rapid Communications 37, 1060 (2016).

124 Dielectric relaxations in poly(glycidyl phenyl ether): effects of microstructure and cyclic topology.

Gambino T, de Ilarduya AM, Alegria A, and Barroso-Bujans F. Macromolecules 49, 1060 (2016).

125 Single chain dynamic structure factor of linear polymers in an all-polymer nano-composite.

Arbe A, Pomposo JA, Asenjo-Sanz I, Bhowmik D, Ivanova O, Kohlbrecher J, and Colmenero J. Macromolecules 49, 2354 (2016).

126 Role of dynamic asymmetry on the collective dynamics of comblike polymers: insights from neutron spin-echo experiments and coarse-grained molecular dynamics simulations.

Arbe A, Moreno AJ, Allgaier J, Ivanova O, Fouquet P, Colmenero J, and Richter D. Macromolecules 49, 4989 (2016).

127 Dynamics and structure of poly(ethylene oxide) intercalated in the nanopores of resorcinol-formaldehyde resin nanoparticles.

Barroso-Bujans F, Cervený S, Palomino P, Enciso E, Rudic S, Fernandez-Alonso F, Alegria A, and Colmenero J. Macromolecules 49, 5704 (2016).

128 Merging of zwitterionic ROP and photoactivated thiol-yne coupling for the synthesis of polyether single-chain nanoparticles.

Rubio-Cervilla J, Barroso-Bujans F, and Pomposo, JA. Macromolecules 49, 90 (2016).

129 **Influence of upconversion processes in the optically-induced inhomogeneous thermal behavior of erbium-doped lanthanum oxysulfide powders.**

Balda R, Hakmeh N, Barredo-Zuriarrain M, Merdrignac-Conanec O, Garcia-Revilla S, Arriandiaga MA, Fernandez J. *Materials* 9, 353 (2016).

130 **Dielectric relaxation analysis of hybrid acrylic-polyurethane gels.**

Martínez-Rugieroa G, Alegría A, Arbe A, Daniloska V, and Colmenero J. *Materials Today Communications* 8, 100 (2016).

131 **Bonding description of the Harpoon mechanism.**

Rodríguez-Mayorga M, Ramos-Cordoba E, Salvador P, Solà M, and Matito E. *Molecular Physics* 114, 1345 (2016).

132 **Similarity measures between excited singlet and triplet electron densities in linear acenes: an application to singlet fission.**

Montero-Cabrera LA, Perez-Badell Y, Piris M, Montero-Alejo AL, de la Vega JMG, and Varandas AJC. *Molecular Physics* 114, 3650 (2016).

133 **Interplay between steps and oxygen vacancies on curved TiO₂(110).**

Miccio LA, Setvin M, Muller M, Abadia M, Piquero I, Lobo-Checa J, Schiller F, Rogero C, Schmid M, Sanchez-Portal D, Diebold U, and Ortega JE. *Nano Letters* 16, 2017 (2016).

134 **Anisotropic nanoantenna-based magnetoplasmonic crystals for highly enhanced and tunable magneto-optical activity.**

Maccaferri N, Bergamini L, Pancaldi M, Schmidt MK, Kataja M, van Dijken S, Zabala N, Aizpurua J, and Vavassori P. *Nano Letters* 16, 2533 (2016).

135 **Manipulating the topological interface by molecular adsorbates: adsorption of Co-Phthalocyanine on Bi₂Se₃.**

Caputo M, Panighel M, Lisi S, Khalil L, Di Santo G, Papalazarou E, Hruban A, Konczykowski M, Krusin-Elbaum L, Aliev ZS, Babanly MB, Otrokov MM, Politano A, Chulkov EV, Arnau A, Marinova V, Das PK, Fujii J, Vobornik I, Perfetti L, Mugarza A, Goldoni A, and Marsi M. *Nano Letters* 16, 3409 (2016).

136 **High temperature ferromagnetism in a GdAg₂ monolayer.**

Ormaza M, Fernandez L, Ilyn M, Magana A, Xu B, Verstraete MJ, Gastaldo M, Valbuena MA, Gargiani P, Mugarza A, Ayuela A, Vitali L, Blanco-Rey M, Schiller F, and Ortega JE. *Nano Letters* 16, 4230 (2016).

137 **Large-scale sublattice asymmetry in pure and boron-doped graphene.**

Usachov DY, Fedorov AV, Vilkov OY, Petukhov AE, Rybkin AG, Ernst A, Otrokov MM, Chulkov EV, Ogorodnikov II, Kuznetsov MV, Yashina LV, Kataev EY, Erofeevskaya AV, Voroshnin VY, Adamchuk VK, Laubschat C, and Vyalikh DV. *Nano Letters* 16, 4535 (2016).

138 **Reversible 2D phase transition driven by an electric field: visualization and control on the atomic scale.**

Wortmann B, van Vorden D, Graf P, Robles R, Abufager P, Lorente N, Bobisch CA, and Müller R. *Nano Letters* 16, 528 (2016).

139 **Tracking optical welding through groove modes in plasmonic nanocavities.**

Mertens J, Demetriadou A, Bowman RW, Benz F, Kleemann ME, Tserkezis C, Shi Y, Yang HY, Hess O, Aizpurua J, and Baumberg JJ. *Nano Letters* 16, 5605 (2016).

140 **On-surface engineering of a magnetic organometallic nanowire.**

Ormaza M, Robles R, Bachellier N, Abufager P, Lorente N, and Limot L. *Nano Letters* 16, 588 (2016).

141 **Real-space mapping of the chiral near-field distributions in spiral antennas and planar metasurfaces.**

Schnell M, Sarriugarte P, Neuman T, Khanikaev AB, Shvets G, Aizpurua J, and Hillenbrand R. *Nano Letters* 16, 663 (2016).

142 **Plasma-wave terahertz detection mediated by topological insulators surface states.**

Viti L, Coquillat D, Politano A, Kokh KA, Aliev ZS, Babanly MB, Tereshchenko OE, Knap W, Chulkov EV, and Vitiello MS. *Nano Letters* 16, 80 (2016).

143 **Optical torques on upconverting particles for intracellular microrheometry.**

Rodríguez-Sevilla P, Zhang YH, de Sousa N, Marques MI, Sanz-Rodríguez F, Jaque D, Liu XG, and Haro-Gonzalez P. *Nano Letters* 16, 8005 (2016).

144 **Plasmon-assisted Nd³⁺-based solid-state nanolaser.**

Molina P, Yraola E, Ramirez MO, Tserkezis C, Plaza JL, Aizpurua J, Bravo-Abad J, and Bausa LE. *Nano Letters* 16, 895 (2016).

145 **Indentation fracture toughness of single-crystal Bi₂Te₃ topological insulators.**

Lamuta C, Cupolillo A, Politano A, Aliev ZS, Babanly MB, Chulkov EV, and Pagnotta L. *Nano Research* 9, 1032 (2016).

146 **Negative dissipation gradients in hysteretic materials.**

Jaafar M, Iglesias-Freire O, Garcia-Mochales P, Sáenz JJ, and Asenjo A. *Nanoscale* 8, 16989 (2016).

147 **Strain-induced effects in the electronic and spin properties of a monolayer of ferromagnetic GdAg₂.**

Correa A, Xu B, Verstraete MJ, and Vitali L. *Nanoscale* 8, 19148 (2016).

148 Existence of nontrivial topologically protected states at grain boundaries in bilayer graphene: signatures and electrical switching.

Jaskolski W, Pelc M, Chico L, and Ayuela A.
Nanoscale 8, 6079 (2016).

149 Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system.

Errea I, Calandra M, Ickard CJP, Nelson JR, Needs RJ, Li YW, Liu HY, Zhang YW, Ma YM, and Mauri F.
Nature 532, 81 (2016).

150 Imaging single-molecule reaction intermediates stabilized by surface dissipation and entropy.

Riss A, Paz AP, Wickenburg S, Tsai HZ, De Oteyza DG, Bradley AJ, Ugeda M, Gorman P, Jung HS, Crommie MF, Rubio A, and Fischer FR.
Nature Chemistry 8, 678 (2016).

151 Force-induced tautomerization in a single molecule.

Ladenthin JN, Frederiksen T, Persson M, Sharp JC, Gawinkowski S, Waluk J, and Kumagai T.
Nature Chemistry 8, 935 (2016).

152 ARPES view on surface and bulk hybridization phenomena in the antiferromagnetic Kondo lattice CeRh₂Si₂.

Patil S, Generalov A, Guttler M, Kushwaha P, Chikina A, Kummer K, Rodel TC, Santander-Syro AF, Caroca-Canales N, Geibel C, Danzenbacher S, Kucherenko Y, Laubschat C, Allen JW, and Vyalikh DV.
Nature Communications 7, 11029 (2016).

153 Quantum mechanical effects in plasmonic structures with subnanometre gaps.

Zhu WQ, Esteban R, Borisov AG, Baumberg JJ, Nordlander P, Lezec HJ, Aizpurua J, and Crozier KB.
Nature Communications 7, 11495 (2016).

154 Spin-texture inversion in the giant Rashba semiconductor BiTeI.

Maass H, Bentmann H, Seibel C, Tusche C, Ereemeev SV, Peixoto TRF, Tereshchenko OE, Kokh KA, Chulkov EV, Kirschner J, and Reinert F.
Nature Communications 7, 11621 (2016).

155 Dynamic spin filtering at the Co/Alq₃ interface mediated by weakly coupled second layer molecules.

Droghetti A, Thielen P, Rungger I, Haag N, Grossmann N, Stöckl J, Stadtmüller B, Aeschlimann M, Sanvito S and Cinchetti M.
Nature Communications 7, 12668 (2016).

156 Suppressing photochemical reactions with quantized light fields.

Galego J, Garcia-Vidal FJ, and Feist J.
Nature Communications 7, 13841 (2016).

157 Ultrafast electronic response of graphene to a strong and localized electric field.

Gruber E, Wilhelm RA, Petuya R, Smejkal V, Kozubek R, Hierzenberger A, Bayer BC, Aldazabal I, Kazansky AK, Libisch F, Krasheninnikov AV, Schleberger M, Facsko S, Borisov AG, Arnau A, and Aumayr F.
Nature Communications 7, 13948 (2016).

158 Quantifying electronic band interactions in van der Waals materials using angle-resolved reflected-electron spectroscopy.

Jobst J, van der Torren AJH, Krasovskii EE, Balgley J, Dean CR, Tromp RM, and van der Molen SJ.
Nature Communications 7, 13621 (2016).

159 Confined linear carbon chains as a route to bulk carbyne.

Shi L, Rohringer P, Suenaga K, Niimi Y, Kotakoski J, Meyer JC, Peterlik H, Wanko M, Cahangirov S, Rubio A, Lapin ZJ, Novotny L, Ayala P, and Pichler T.
Nature Materials 15, 634 (2016).

160 The omega-SQUIPT as a tool to phase-engineer Josephson topological materials.

Strambini E, D'Ambrosio S, Vischi F, Bergeret FS, Nazarov YV, and Giazotto F.
Nature Nanotechnology 11, 1055 (2016).

161 NANOCAVITIES optomechanics goes molecular.

Schmidt MK, and Aizpurua J.
Nature Nanotechnology 11, 114 (2016).

162 Efficiency of dopant-induced ignition of helium nanoplasmas.

Heidenreich A, Gruner B, Rometsch M, Krishnan SR, Stienkemeier F, and Mudrich M.
New Journal of Physics 18, 073046 (2016).

163 Negative plasmon dispersion in 2H-NbS₂ beyond the charge-density-wave interpretation.

Cudazzo P, Muller E, Habenicht C, Gatti M, Berger H, Knupfer M, Rubio A, and Huotari S.
New Journal of Physics 18, 103050 (2016).

164 Pressure effects on crystal and electronic structure of bismuth tellurohalides.

Rusinov IP, Menshchikova TV, Sklyadneva IY, Heid R, Bohnen KP, and Chulkov EV.
New Journal of Physics 18, 1367 (2016).

165 Energy loss in gas-surface dynamics: electron-hole pair and phonon excitation upon adsorbate relaxation.

Novko D, Blanco-Rey M, Juaristi JI, and Alducin M.
Nuclear Instruments & Methods in Physics Research B 382, 26 (2016).

166 Density functional theory study of nitrogen atoms and molecules interacting with Fe(111) surfaces.

Nosir MA, Martin-Gondre L, Bocan GA, and Muino RD.
Nuclear Instruments and Methods in Physics Research B 382, 105 (2016).

167 Femtosecond laser pulse induced desorption: A molecular dynamics simulation.

Loncaric I, Alducin M, Saalfrank P, and Juaristi JI.
Nuclear Instruments and Methods in Physics Research B 382, 114 (2016).

168 Quantum effects in the plasmon response of bimetallic core-shell nanostructures.

Marinica DC, Aizpurua J, and Borisov AG.
Optics Express 24, 23941 (2016).

- 169 **Strong coupling between phonon-polaritons and plasmonic nanorods.**
Huck C, Vogt J, Neuman T, Nagao T, Hillenbrand R, Aizpurua J, Pucci A, and Neubrech F.
Optics Express 24, 25528 (2016).
- 170 **Plasmonic enhancement of second harmonic generation from nonlinear RbTiOPO₄ crystals by aggregates of silver nanostructures.**
Sanchez-Garcia L, Tserkezis C, Ramirez MO, Molina P, Carvajal JJ, Aguiló M, Diaz F, Aizpurua J, and Bausa LE.
Optics Express 24, 8491 (2016).
- 171 **Chiroptical activity in colloidal quantum dots coated with achiral ligands.**
Melnikau D, Savateeva D, Gaponik N, Govorov AO, and Rakovich YP.
Optics Express 24, A65 (2016).
- 172 **A useful methodology for determining the compaction degree of single-chain nanoparticles by conventional SEC.**
Latorre-Sanchez A, Alegria A, Lo Verso F, Moreno AJ, Arbe A, Colmenero J, and Pomposo JA.
Particle & Particle Systems Characterization 33, 373 (2016).
- 173 **Proposed sets of critical exponents for randomly branched polymers, using a known string theory model.**
March NH, and Moreno AJ.
Phase Transitions 89, 543 (2016).
- 174 **Nanoindentation of single-crystal Bi₂Te₃ topological insulators grown with the Bridgman-Stockbarger method.**
Lamuta C, Cupolillo A, Politano A, Aliev ZS, Babanly MB, Chulkov EV, Alfano M, and Pagnotta L.
Physica Status Solidi B-Basic Solid State Physics 253, 1082 (2016).
- 175 **An electronic aromaticity index for large rings.**
Matito E.
Physical Chemistry Chemical Physics 18, 11839 (2016).
- 176 **The stability of biradicaloid versus closed-shell [E(μ -XR)]₂ (E = P, As; X = N, P, As) rings. Does aromaticity play a role?**
Grande-Aztatzi R, Mercero JM, and Ugalde JM.
Physical Chemistry Chemical Physics 18, 11879 (2016).
- 177 **Dihydrogen bond interactions as a result of H-2 cleavage at Cu, Ag and Au centres.**
Grabowski SJ, and Ruiperez F.
Physical Chemistry Chemical Physics 18, 12810 (2016).
- 178 **Complexes of carborane acids linked by strong hydrogen bonds: acidity scales.**
Grabowski SJ.
Physical Chemistry Chemical Physics 18, 16152 (2016).
- 179 **Diels-Alder attachment of a planar organic molecule to a dangling bond dimer on a hydrogenated semiconductor surface.**
Godlewski S, Kawai H, Engelund M, Kolmer M, Zuzak R, Garcia-Lekue A, Novell-Leruth G, Echavarren AM, Sanchez-Portal D, Joachim C, and Saeys M.
Physical Chemistry Chemical Physics 18, 16757 (2016).
- 180 **Design of new disulfide-based organic compounds for the improvement of self-healing materials.**
Matxain JM, Asua JM, and Ruiperez F.
Physical Chemistry Chemical Physics 18, 1758 (2016).
- 181 **The butterfly - a well-defined constant-current topography pattern on Si(001):H and Ge(001):H resulting from current-induced defect fluctuations.**
Engelund M, Godlewski S, Kolmer M, Zuzak R, Such B, Frederiksen T, Szymonski M, and Sanchez-Portal D.
Physical Chemistry Chemical Physics 18, 19309 (2016).
- 182 **Substitutional 4d and 5d impurities in graphene.**
Alonso-Lanza T, Ayuela A, and Aguilera Granja F.
Physical Chemistry Chemical Physics 18, 21913 (2016).
- 183 **Separation of dynamic and nondynamic correlation.**
Ramos-Cordoba E, Salvador P, and Matito E.
Physical chemistry chemical physics 18, 24015 (2016).
- 184 **Molecular dynamics simulation of O-2 adsorption on Ag(110) from first principles electronic structure calculations.**
Loncaric I, Alducin M, and Juaristi JI.
Physical Chemistry Chemical Physics 18, 27366 (2016).
- 185 **A redox-active radical as an effective nanoelectronic component: stability and electrochemical tunnelling spectroscopy in ionic liquids.**
Rudnev AV, Franco C, Crivillers N, Seber G, Droghetti A, Rungger I, Pobelov IV, Veciana J, Mas-Torrent M, and Rovira C.
Physical Chemistry Chemical Physics 18, 27733 (2016).
- 186 **A computational study of radical initiated protein backbone homolytic dissociation on all natural amino acids.**
Uranga J, Lakuntza O, Ramos-Cordoba Eloy, Matxain JM, and Mujika JI.
Physical Chemistry Chemical Physics 18, 30972 (2016).
- 187 **Hydrogen abstraction from metal surfaces: when electron-hole pair excitations strongly affect hot-atom recombination.**
Galparsoro O, Petuya R, Busnengo HF, Juaristi JI, Crespos C, Alducin M, and Larregaray P.
Physical Chemistry Chemical Physics 18, 31378 (2016).

188 **Interaction of a conjugated polyaromatic molecule with a single dangling bond quantum dot on a hydrogenated semiconductor.**

Godlewski S, Kolmer M, Engelund M, Kawai H, Zuzak R, Garcia-Lekue A, Saeys M, Echavarren AM, Joachim C, Sanchez-Portal D, and Szymonski M.
Physical Chemistry Chemical Physics 18, 3854 (2016).

189 **Phosphorylation promotes Al(III) binding to proteins: GEGEGSGG as a case study.**

Grande-Aztatzi R, Formoso E, Mujika JI, Ugalde JM, and Lopez X.
Physical Chemistry Chemical Physics 18, 7197 (2016).

190 **NO adsorption on Cu(110) and O(2 * 1)/Cu(110) surfaces from density functional theory calculations.**

Brion-Rios AX, Sanchez-Portal D, and Cabrera-Sanfeliix P.
Physical Chemistry Chemical Physics 18, 9476 (2016).

191 **Interference effects in angular streaking with a rotating terahertz field.**

Kazansky AK, Bozhevolnov AV, Sazhina IP, and Kabachnik NM.
Physical Review A 93, 013407 (2016).

192 **Fluctuations of the electromagnetic local density of states as a probe for structural phase switching.**

de Sousa N, Saenz JJ, Scheffold F, Garcia-Martin A, and Froufe-Perez LS.
Physical Review A 94, 043832 (2016).

193 **Nonreciprocal few-photon routing schemes based on chiral waveguide-emitter couplings.**

Gonzalez-Ballesteros C, Moreno E, Garcia-Vidal FJ, and Gonzalez-Tudela A.
Physical Review A 94, 063817 (2016).

194 **Role of valence states of adsorbates in inelastic electron tunneling spectroscopy: A study of nitric oxide on Cu(110) and Cu(001).**

Shiotari A, Okuyama H, Hatta S, Aruga T, Alducin M, and Frederiksen T.
Physical Review B 92, 075442 (2016).

195 **Surface electron density models for accurate ab initio molecular dynamics with electronic friction.**

Novko D, Blanco-Rey M, Alducin M, and Juaristi JI.
Physical Review B 92, 245435-1 (2016).

196 **Femtosecond-laser-driven molecular dynamics on surfaces: photodesorption of molecular oxygen from Ag(110).**

Loncaric I, Alducin M, Saalfrank P, and Juaristi JI.
Physical Review B 93, 014301 (2016).

197 **Origin of inverse Rashba-Edelstein effect detected at the Cu/Bi interface using lateral spin valves.**

Isasa M, Martinez-Velarte MC, Villamor E, Magen C, Morellon L, De Teresa JM, Ibarra MR, Vignale G, Chulkov EV, Krasovskii EE, and Hueso LE.
Physical Review B 93, 014420 (2016).

198 **Stimulated quasiparticles in spin-split superconductors.**

Virtanen P, Heikkila TT, and Bergeret FS.
Physical Review B 93, 014512 (2016).

199 **Dissociation products and structures of solid H₂S at strong compression.**

Li YW, Wang L, Liu HY, Zhang YW, Hao J, Pickard CJ, Nelson JR, Needs RJ, Li WT, Huang YW, Errea I, Calandra M, Mauri F, and Ma YM.
Physical Review B 93, 020103 (2016).

200 **Theory of the nonlinear Rashba-Edelstein effect: The clean electron gas limit.**

Vignale G, and Tokatly IV.
Physical Review B 93, 035310 (2016).

201 **Role of the kinematics of probing electrons in electron energy-loss spectroscopy of solid surfaces.**

Nazarov VU, Silkin VM, and Krasovskii EE.
Physical Review B 93, 035403 (2016).

202 **Plasmon dissipation in gapped graphene open systems at finite temperature.**

Iurov A, Gumbs G, Huang D, and Silkin VM.
Physical Review B 93, 035404 (2016).

203 **Engineering the emission of light from a scanning tunneling microscope using the plasmonic modes of a nanoparticle.**

Le Moal E, Marguet S, Cannesson D, Rogez B, Boer-Duchemin E, Dujardin G, Teperik TV, Marinica DC, and Borisov AG.
Physical Review B 93, 035418 (2016).

204 **Dielectric screening and plasmon resonances in bilayer graphene.**

Pisarra M, Sindona A, Gravina M, Silkin VM, and Pitarke JM.
Physical Review B 93, 035440 (2016).

205 **Nonequilibrium plasmon emission drives ultrafast carrier relaxation dynamics in photoexcited graphene.**

Hamm JM, Page AF, Bravo-Abad J, Garcia-Vidal FJ, and Hess O.
Physical Review B 93, 041408(R) (2016).

206 **Spin texture induced by oxygen vacancies in strontium perovskite (001) surfaces: a theoretical comparison between SrTiO₃ and SrHfO₃.**

Garcia-Castro AC, Vergniory MG, Bousquet E, and Romero AH.
Physical Review B 93, 045405 (2016).

207 **Relaxation of the resistive superconducting state in boron-doped diamond films.**

Kardakova A, Shishkin A, Semenov A, Goltsman GN, Ryabchun S, Klapwijk TM, Bousquet J, Eon D, Sacepe B, Klein T, and Bustarret E.
Physical Review B 93, 064506 (2016).

208 **Low-coverage surface diffusion in complex periodic energy landscapes: analytical solution for systems with symmetric hops and application to intercalation in topological insulators.**
Gosalvez MA, Otrokov MM, Ferrando N, Ryabishchenkova AG, Ayuela A, Echenique PM, and Chulkov EV.
Physical Review B 93, 075429 (2016).

209 **New family of graphene-based organic semiconductors: An investigation of photon-induced electronic structure manipulation in half-fluorinated graphene.**
Walter AL, Sahin H, Kang J, Jeon KJ, Bostwick A, Horzum S, Moreschini L, Chang YJ, Peeters FM, Horn K, and Rotenberg E.
Physical Review B 93, 075439 (2016).

210 **Extrinsic spin Hall effect from anisotropic Rashba spin-orbit coupling in graphene.**
Yang HY, Huang CL, Ochoa H, and Casalilla, MA.
Physical Review B 93, 085418 (2016).

211 **Highly anisotropic thermal conductivity of arsenene: an ab initio study.**
Zeraati M, Allaei SMV, Sarsari IA, Pourfath M, and Donadio D.
Physical Review B 93, 085424 (2016).

212 **Ab initio calculation of the shock Hugoniot of bulk silicon.**
Strickson O, and Artacho E.
Physical Review B 93, 094107 (2016).

213 **Vacancy-induced flow of solid helium.**
Benedek G, Kalinin A, Nieto P, and Toennies JP.
Physical Review B 93, 104505 (2016).

214 **Semilocal density functional theory with correct surface asymptotics.**
Constantin LA, Fabiano E, Pitarke JM and Della Sala F.
Physical Review B 93, 115127 (2016).

215 **Bilayer SnS₂: Tunable stacking sequence by charging and loading pressure.**
Bacaksiz C, Cahangirov S, Rubio A, Senger RT, Peeters FM, and Sahin H.
Physical Review B 93, 125403 (2016).

216 **Optical absorption and conductivity in quasi-two-dimensional crystals from first principles: application to graphene.**
Novko D, Sunjic M, and Despoja V.
Physical Review B 93, 125413 (2016).

217 **Electron tunneling through water layer in nanogaps probed by plasmon resonances.**
Teperik TV, Kazansky AK, and Borisov AG.
Physical Review B 93, 155431 (2016).

218 **Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability.**
Borinaga M, Errea I, Calandra M, Mauri F, and Bergara A.
Physical Review B 93, 174308 (2016).

219 **Orbital magnetization in insulators: Bulk versus surface.**
Bianco R, and Resta R.
Physical Review B 93, 174417 (2016).

220 **Fundamental gap of molecular crystals via constrained density functional theory.**
Droghetti A, Rungger I, Das Pemmaraju C, and Sanvito S.
Physical Review B 93, 195208 (2016).

221 **Low-coverage surface diffusion in complex periodic energy landscapes: II. Analytical solution for systems with asymmetric hops.**
Gosalvez MA, Otrokov MM, Ferrando N, Ryabishchenkova AG, Ayuela A, Echenique PM, and Chulkov EV.
Physical Review B 93, 205416 (2016).

222 **Attosecond and femtosecond forces exerted on gold nanoparticles induced by swift electrons.**
Lagos MJ, Reyes-Coronado A, Konecna A Echenique PM, Aizpurua J, and Batson PE.
Physical Review B 93, 205440 (2016).

223 **Lieb-Mattis ferrimagnetism in magnetic semiconductors.**
Kuzian RO, Richter J, Kuz'min MD, and Hayn R.
Physical Review B 93, 214433 (2016).

224 **Stable Dirac semimetal in the allotropes of group-IV elements.**
Cao WD, Tang PZ, Zhang SC, Duan WH, and Rubio A.
Physical Review B 93, 241117 (2016).

225 **Observation of a charge delocalization from Se vacancies in Bi₂Se₃: A positron annihilation study of native defects.**
Unzueta I, Zabala N, Marin-Borras V, Munoz-Sanjose V, Garcia JA, and Plazaola F.
Physical Review B 94, 014117 (2016).

226 **Ballistic Josephson junctions in the presence of generic spin dependent fields.**
Konschelle F, Tokatly IV, and Bergeret FS.
Physical Review B 94, 014515 (2016).

227 **Extremely long-lived magnetic excitations in supported Fe chains.**
Gauyacq JP, and Lorente N.
Physical Review B 94, 045420 (2016).

228 **Structural and magnetic properties of FeM_x chains (x=1-6) supported on Cu₂N/Cu (100).**
Choi DJ, Robles R, Gauyacq JP, Ternes M, Loth S, and Lorente N.
Physical Review B 94, 085406 (2016).

229 **Direct coupling between charge current and spin polarization by extrinsic mechanisms in graphene.**
Chunli H, Chong YD, and Casalilla MA.
Physical Review B 94, 085414 (2016).

230 **One-step approach to ARPES from strongly correlated solids: A Mott-Hubbard system.**

Kuzian RO, and Krasovskii EE.
Physical Review B 94, 115119 (2016).

231 **Dissipative long-range entanglement generation between electronic spins.**

Benito M, Schuetz MJA, Cirac JI, Platero G, and Giedke G.
Physical Review B 94, 115404 (2016).

232 **Optical absorption and transmission in a molybdenum disulfide monolayer.**

Rukelj Z, Strkalj A, and Despoja V.
Physical Review B 94, 115428 (2016).

233 **Formation of the BiAg₂ surface alloy on lattice-mismatched interfaces.**

Abd El-Fattah ZM, Lutz P, Piquero-Zulaica I, Lobo-Checa J, Schiller F, Bentmann H, Ortega JE, and Reinert F.
Physical Review B 94, 155447 (2016).

234 **Adsorption geometry and electronic properties of flat-lying monolayers of tetracene on the Ag(111) surface.**

Zaitsev NL, Nechaev IA, Hofer U, and Chulkov EV.
Physical Review B 94, 155452 (2016).

235 **Surface Fermi arc connectivity in the type-II Weyl semimetal candidate WTe₂.**

Sanchez-Barriga J, Vergniory MG, Evtushinsky D, Aguilera I, Varykhalov A, Bluel S, and Rader O.
Physical Review B 94, 161401 (2016).

236 **Temperature effect on acoustic plasmons.**

Silkin VM, Nazarov VU, Balassis A, Chernov IP, and Chulkov EV.
Physical Review B 94, 165122 (2016).

237 **Kernel-corrected random-phase approximation for the uniform electron gas and jellium surface energy.**

Ruzsinszky A, Constantin LA, and Pitarke JM.
Physical Review B 94, 165155 (2016).

238 **Noncontact atomic force microscopy and density functional theory studies of the (2 x 2) reconstructions of the polar AlN(0001) surface.**

Chaumeton F, Robles R, Pruneda M, Lorente N, Eydoux B, Bouju X, Gauthier S, and Martrou D.
Physical Review B 94, 165305 (2016).

239 **Femtosecond-laser induced dynamics of CO on Ru(0001): deep insights from a hot-electron friction model including surface motion.**

Scholz R, Floss G, Saalfrank P, Fuchsel G, Loncaric I, and Juaristi JI.
Physical Review B 94, 165447 (2016).

240 **Manifestation of extrinsic spin Hall effect in superconducting structures: Nondissipative magnetoelectric effects.**

Bergeret FS, and Tokatly IV.
Physical Review B 94, 180502 (2016).

241 **When polarons meet polaritons: Exciton-vibration interactions in organic molecules strongly coupled to confined light fields.**

Wu N, Feist J, and Garcia-Vidal FJ.
Physical Review B 94, 195409 (2016).

242 **Polyyne electronic and vibrational properties under environmental interactions.**

Wanko M, Cahangirov S, Shi L, Rohringer P, Lapin ZJ, Novotny L, Ayala P, Pichler T, and Rubio A.
Physical Review B 94, 195422 (2016).

243 **Rapid propagation of a Bloch wave packet excited by a femtosecond ultraviolet pulse.**

Krasovskii EE, Friedrich C, Schattke W, and Echenique PM.
Physical Review B 94, 195434 (2016).

244 **Relativistic $k \cdot p$ Hamiltonians for centrosymmetric topological insulators from ab initio wave functions.**

Nechaev IA, and Krasovskii EE.
Physical Review B 94, 201410 (2016).

245 **Effects of electronic relaxation processes on vibrational linewidths of adsorbates on surfaces: The case of CO/Cu(100).**

Novko D, Alducin M, Blanco-Rey M, and Juaristi JI.
Physical Review B 94, 224306 (2016).

246 **An array of layers in silicon sulfides: chainlike and monolayer.**

Alonso-Lanza T, Ayuela A, and Aguilera-Granja F.
Physical Review B 94, 245441 (2016).

247 **Control of diffusion of nanoparticles in an optical vortex lattice.**

Zapata I, Delgado-Buscalioni R, and Saenz JJ.
Physical Review E 93, 062130 (2016).

248 **Continuous melting through a hexatic phase in confined bilayer water.**

Zubeltzu J, Corsetti F, Fernandez-Serra MV, and Artacho E.
Physical Review E 93, 062137 (2016).

249 **Hanle magnetoresistance in thin metal films with strong spin-orbit coupling.**

Velez S, Golovach VN, Bedoya-Pinto A, Isasa M, Sagasta E, Abadia M, Rogero C, Hueso LE, Bergeret FS, and Casanova F.
Physical Review Letters 116, 016603 (2016).

250 **Enhanced configurational entropy in high-density nanoconfined bilayer ice.**

Corsetti F, Zubeltzu J, and Artacho E.
Physical Review Letters 116, 085901 (2016).

251 **Irrelevance of the boundary on the magnetization of metals.**

Marrazzo A, and Resta R.

Physical Review Letters 116, 137201 (2016).

252 **Semiclassical quantization of spinning quasiparticles in ballistic Josephson junctions.**

Konschelle F, Bergeret FS, and Tokatly IV.

Physical Review Letters 116, 237002 (2016).

253 **Transformation optics approach to plasmon-exciton strong coupling in nanocavities.**

Li RQ, Hernangomez-Perez D, Garcıa-Vidal FJ, and Fernandez-Domınguez AI.

Physical Review Letters 117, 107401 (2016).

254 **Plasmon modes of graphene nanoribbons with periodic planar arrangements.**

Gomez CV, Pisarra M, Gravina M, Pitarke JM, and Sindona A.

Physical Review Letters 117, 116801 (2016).

255 **Uncoupled dark states can inherit polaritonic properties.**

Gonzalez-Ballester C, Feist J, Gonzalo Badıa E, Moreno E, and Garcia-Vidal FJ.

Physical Review Letters 117, 156402 (2016).

256 **Time-reversal-breaking weyl fermions in magnetic heusler alloys.**

Wang ZJ, Vergniory MG, Kushwaha S, Hirschberger M, Chulkov EV, Ernst A, Ong NP, Cava RJ, and Bernevig, BA.

Physical Review Letters 117, 236401 (2016).

257 **Exploiting vibrational strong coupling to make an optical parametric oscillator out of a raman laser.**

del Pino J, Garcia-Vidal FJ, and Feist J.

Physical Review Letters 117, 277401 (2016).

258 **Dielectric susceptibility of liquid water: microscopic insights from coherent and incoherent neutron scattering.**

Arbe A, Malo de Molina P, Alvarez F, Frick B, and Colmenero J.

Physical Review Letters 117, 5501 (2016).

259 **Hidden string order in a hole superconductor with extended correlated hopping.**

Chhajlany RW, Grzybowski PR, Stasinska J, Lewenstein M, and Dutta O.

Physical Review Letters, 116, 225303 (2016).

260 **Unified theory of critical exponents generated by the Ising Hamiltonian for discrete dimensionalities 2, 3 and 4 in terms of the critical exponent h.**

March NH.

Physics and Chemistry of Liquids 54, 127 (2016).

261 **Potential energy curves for P-2 and P-2(+) constructed from a strictly N-representable natural orbital functional.**

Piris M, and March NH.

Physics and Chemistry of Liquids 54, 797 (2016).

262 **Novel effects of strains in graphene and other two dimensional materials.**

Amorim B, Cortijo A, de Juan F, Grushine AG, Guinea F, Gutierrez-Rubio A, Ochoa H, Parente V, Roldan R, San-Jose P, Schiefele J, Sturla M, and Vozmediano MAH.

Physics Reports-Review Section of Physics Letters 617, 1 (2016).

263 **Structure and dynamics of single-chain nano-particles in solution.**

Arbe A, Pomposo JA, Moreno AJ, LoVerso F, Gonzalez-Burgos M, Asenjo-Sanz I, Iturrospe A, Radulescu A, Ivanova O, and Colmenero J.

Polymer 105, 532 (2016).

264 **An unexpected route to aldehyde-decorated single-chain nanoparticles from azides.**

Gonzalez-Burgos M, Alegria A, Arbe A, Colmenero J, and Pomposo, JA.

Polymer Chemistry 7, 6570 (2016).

265 **Effect of nanostructure on the thermal glass transition and physical aging in polymer materials.**

Cangialosi D, Alegria A, and Colmenero J.

Progress in Polymer Science 54, 128 (2016).

266 **Circular dichroism measurements at an x-ray free-electron laser with polarization control.**

Hartmann G, Lindahl AO, Knie A, Hartmann N, Lutman AA, MacArthur JP, Shevchuk I, Buck J, Galler A, Glownia JM, Helml W, Huang Z, Kabachnik NM, Kazansky AK, Liu J, Marinelli A, Mazza T, Nuhn HD, Walter P, Viefhaus J, Meyer M, Moeller S, Coffee RN, and Ilche M.

Review of scientific instruments 87, 083113 (2016).

267 **Permanent excimer superstructures by supramolecular networking of metal quantum clusters.**

Santiago-Gonzalez B, Monguzzi A, Azpiroz JM, Prato M, Erratico S, Campione M, Lorenzi R,

Pedrini J, Santambrogio C, Torrente Y, De Angelis F, Meinardi F, and Brovelli S.

Science 353, 571 (2016).

268 **Beyond Dirac and Weyl fermions: Unconventional quasiparticles in conventional crystals.**

Bradlyn B, Cano J, Wang ZJ, Vergniory MG, Felser C, Cava RJ, and Bernevig BA.

Science 353, 6299 (2016).

269 **Single-molecule optomechanics in "picocavities".**

Benz F, Schmidt MK, Dreismann A, Chikkaraddy R, Zhang Y, Demetriadou A, Carnegie C,

Ohadi H, de Nijs B, Esteban R, Aizpurua J, and Baumberg JJ.

Science 354, 726 (2016).

270 **Structural and configurational properties of nanoconfined monolayer ice from first principles.**

Corsetti F, Matthews P, and Artacho E.

Scientific Reports 6, 18651 (2016).

271 **Mirror-symmetry protected non-TRIM surface state in the weak topological insulator Bi₂Tel.**

Rusinov IP, Menshchikova TV, Isaeva A, Ereemeev SV, Koroteev YM, Vergniory MG, Echenique PM, and Chulkov EV.

Scientific Reports 6, 20734 (2016).

272 **Plasmon excitations of multilayer graphene on a conducting substrate.**

Gumbs G, Iurov A, Wu JY, Lin MF, and Fekete P.
Scientific Reports 6, 21063 (2016).

273 **Topological crystalline insulator in a new Bi semiconducting phase.**

Munoz F, Vergniory MG, Rauch T, Henk J, Chulkov EV, Mertig I, Botti S, Marques MAL, and Romero AH.
Scientific Reports 6, 21790 (2016).

274 **Pressure-induced topological phases of KNa₂Bi.**

Sklyadneva IYu, Rusinov IP, Heid R, Bohnen K-P, Echenique PM, and Chulkov E.
Scientific Reports 6, 24137 (2016).

275 **Robust and tunable itinerant ferromagnetism at the silicon surface of the antiferromagnet GdRh₂Si₂.**

Güttler M, Generalov M, Otrokov MM, Kummer K, Kliemt K, Fedorov A, Chikina A, Danzenbächer S, Schulz S, Chulkov EV, Koroteev Yu.M, Caroca-Canales N, Shi M, Radovic M, Geibel C, Laubschat C, Dudin P, Kim TK, Hoesch M, Krellner C, and Vyalikh DV.
Scientific Reports 6, 24254 (2016).

276 **Magneto-optical activity in high index dielectric nanoantennas.**

de Sousa N, Froufe-Perez LS, Saenz J J, and Garcia-Martin A.
Scientific Reports 6, 30803 (2016).

277 **What is the mechanism of formation of hydroxyaluminosilicates?**

Beardmore J, Lopez X, Mujika, JI, and Exley Ch.
Scientific Reports 6, 30913 (2016).

278 **Temperature-driven topological quantum phase transitions in a phase-change material Ge₂Sb₂Te₅**

Eremeev SV, Rusinov IP, Echenique PM, and Chulkov EV.
Scientific Reports 6, 38799 (2016).

279 **Mechanical properties of Si₂Te₃ topological insulator investigated by density functional theory and nanoindentation.**

Lamuta C, Campi D, Cupolillo A, Aliev ZS, Babanly MB, Chulkov EV, Politano A, and Pagnotta L.
Scripta Materialia 121, 50 (2016).

280 **Monitoring early-stage nanoparticle assembly in microdroplets by optical spectroscopy and SERS.**

Salmon AR, Esteban R, Taylor RW, Hugall JT, Smith CA, Whyte G, Scherman OA, Aizpurua J, Abell C, and Baumberg JJ.
Small 12, 1788 (2016).

281 **Configuring electronic states in an atomically precise array of quantum boxes.**

Nowakowska S, Wäckerlin A, Piquero-Zulaica I, Nowakowski J, Kawai S, Wäckerlin C, Matena M, Nijs T, Fatayer S, Popova O, Ahsan A, Mousavi SF, Ivas T, Meyer E, Stöhr M, Ortega JE, Björk J, Gade LH, and Lobo-Checa J, Jung TA.
Small 12, 3757 (2016).

282 **Anisotropic effective interactions and stack formation in mixtures of semiflexible ring polymers.**

Poier P, Bacova P, Moreno AJ, Likos CN, and Blaak R.
Soft Matter 12, 4805 (2016).

283 **Dielectric relaxation of polymers: segmental dynamics under structural constraints.**

Alegria A, and Colmenero J.
Soft Matter 12, 7709 (2016).

284 **Tunable slow dynamics in a new class of soft colloids.**

Lo Verso F, Pomposo JA, Colmenero J, and Moreno AJ.
Soft Matter 12, 9039 (2016).

285 **Structural, magnetic and optical properties of two concomitant molecular crystals.**

Silva MR, Milne B, Coutinho JT, Pereira LCJ, Martin-Ramos P, da Silva PSP, and Martin-Gil J.
Solid State Sciences 53, 37 (2016).

286 **Resolubility of image-potential resonances.**

Höfer U, and Echenique PM.
Surface Science 643, 203 (2016).

287 **Adsorption of polyiodobenzene molecules on the Pt(111) surface using van der Waals density functional theory.**

Johnston K, Pekoz R, and Donadio D.
Surface Science 644, 113 (2016).

288 **Rotation assisted diffusion of water trimers on Pd(111).**

Ranea VA, and de Andres PL.
Surface Science 648, 256 (2016).

289 **Cyclopropanation reactions catalysed by dendrimers possessing one metalloporphyrin active site at the core: linear and sigmoidal kinetic behaviour for different dendrimer generations.**

Vins P, de Cozar A, Rivilla I, Novakova K, Zangi R, Cvacka J, Arrastia I, Arrieta A, Drasar P, Miranda JI, and Cossio FP.
Tetrahedron 72, 1120 (2016).

290 **Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition.**

Ruiz I, Matito E, Holguin-Gallego FJ, Francisco E, Pendas AM, and Rocha-Rinza T.
Theoretical Chemistry Accounts 135, 209 (2016).

291 **Exact exchange-correlation functional for the infinitely stretched hydrogen molecule.**

Matito E, Casanova D, Lopez X, and Ugalde JM.
Theoretical Chemistry Accounts 135, 226 (2016).

292 **Diversity characterization of binary clusters by means of a generalized distance.**

Ramirez M, Rogan J, Valdivia JA, Varas A, and Kiwi M.
Zeitschrift für Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics 230, 977 (2016).