



Results

DIPC Publications 2006

- Strain and spin-orbit effects in self-assembled quantum dots.
Zielinski M, Jaskolski W, Aizpurua J, Bryant GW.
Acta Physica Polonica A **110**, 443 (2006).
- Synthesis and optical properties of gold nanodecahedra with size control.
Sánchez-Iglesias A, Pastoriza-Santos I, Pérez-Juste J, Rodríguez-González B, García de Abajo FJ, and Liz-Marzán L.
Advanced Materials **18**, 2529 (2006).
- High Curie temperatures in (Ga,Mn)N from Mn clustering.
Hynninen T, Raebiger H, Von Boehm J, and Ayuela A.
Applied Physics Letters **88**, 122501 (2006).
- Resonances of individual metal nanowires in the infrared.
Neubrech F, Kolb T, Lovrincic R, Fahsold G, Puccia A, Aizpurua J, Cornelius TW, Toimil-Molaes ME, Neumann R, and Karim S.
Applied Physics Letters **89**, 253104 (2006).
- Electronic excitations in metal and at metal surfaces.
Chulkov EV, Borisov AG, Gauyacq JP, Sánchez-Portal D, Silkin VM, Zhukov VP, and Echenique PM.
Chemical Review **106**, 4160 (2006).
- Sandwich Complexes Based on the "All-Metal" Al₄ 2- Aromatic Ring Chemistry.
Mercero JM, Formoso E, Matxain JM, Eriksson LA, and Ugalde JM.
Chemistry – A European Journal **12**, 4495 (2006).
- Recent development of multireference density functional theory
Yamanaka S, Nakata K, Takada T, Kusakabe K, Ugalde JM and Yamaguchi K.
Chemistry Letters (Highlight Review) **35**, 242 (2006).
- Resonance structures of the amide bond: the advantages of planarity.
Mujika JI, Matxain JM, Eriksson LA, and Lopez X.
Chemistry – A European Journal **12**, 7215 (2006).
- Density functional study of molecular hydrogen coverage on carbon nanotubes.
Cabria I, López MJ and Alonso JA.
Computational Materials Science **35**, 238 (2006).
- Exact Non-Born-Oppenheimer wave function for the Hooke-Calogero model of the H₂ molecule.
Lopez X, Ugalde, JM and Ludeña EV.
European Journal of Physics D **37**, 351 (2006).
- X-ray photoelectron diffraction study of ultrathin PbTiO₃ films.
Despont L, Lichtensteiger C, Clerc F, Garnier MG, Garcia de Abajo FJ, Van Hove MA, Triscone JM, and Aebi P.
European Physical Journal B **49**, 141 (2006).

Counterintuitive effects of the electron correlation in the first-excited $1\Sigma_g^+$ state of the hydrogen molecule.

Wang J, Mercero JM, Silanes I, and Ugalde JM.
Europhysics Letters **76**, 808 (2006).

No Evidence of Metallic Methane at High Pressure.

Martínez-Canales M, and Bergara A.
High Pressure Research **26**, 369 (2006).

Fermi Surface Deformation in Lithium Under High Pressure.

Rodríguez-Prieto A. and Bergara A.
High Pressure Research **26**, 461 (2006).

Calculation of metastable free-energy diagrams and glass formation in the Mg–Cu–Y alloy and its boundary binaries using the Miedema model.

Hojvat de Tandler R, Soriano MR, Pepe ME, Kovacs JA,
Vicente EE, and Alonso JA.
Intermetallics **14**, 297 (2006).

Feynman propagator and Slater sum for a model Hamiltonian motivated by H-2(+) in an intense magnetic field.

Amovilli C, March NH.
International Journal of Quantum Chemistry **106**, 533 (2006).

Quantum size effects in metallic overlayers.

Zabala N, Ogando E, Chulkov EV, and Puska MJ.
Izvestia RAN (seria fizicheskaya) **70**, 894 (2006).

Optical absorption spectra of V4+ isomers: one example of first-principles theoretical spectroscopy with time-dependent density functional theory.

Martínez JI, Castro A, Rubio A, and Alonso JA.
Journal of Computational and Theoretical Nanoscience **3**, 1 (2006).

A study of the coordination shell of aluminum(III) and magnesium(II) in model protein environments: Thermodynamics of the complex formation and metal exchange reactions.

Rezabal E, Mercero JM, Lopez X and Ugalde JM.
Journal of Inorganic Biochemistry **100**, 374 (2006).

Spectroscopic properties of Yb3+ ions in halogeno-sulfide glasses.

Balda R, Seznec V, Nazabal V, Adam JL, Al-Saleh M, Fernandez J.
Journal of Non-Crystalline Solids **352**, 2444, (2006).

Site selective spectroscopy of Eu3+ in heavy-metal oxide glasses.

Cascales C, Balda R, Fernandez J, Arriandiaga MA, Fdez-Navarro JM.
Journal of Non-Crystalline Solids **352**, 24489 (2006).

Hydrogen dynamics in polyethersulfone: A quasielastic neutron scattering study in the high-momentum transfer region.

Quintana I, Arbe A, Colmenero J, and Frick B.
Journal of Non-Crystalline Solids **352**, 4610 (2006).

Molecular motions in glassy polycarbonate below its glass transition temperature.

Arrese-Igor S, Mitxelena O, A. Arbe A, Alegría A, Colmenero J, and Frick B.
Journal of Non-Crystalline Solids **352**, 5072 (2006).

Self-Assembly of Heterogeneous Supramolecular Structures with Uniaxial Anisotropy.

Ruiz-Osés M, Gonzalez-Lakunza N, Silanes I, Gourdon A, Arnau A,
and Ortega JE.
Journal of Physical Chemistry B **110**, 25573-25577 (2006).

Water Adsorption and Diffusion on NaCl(100).

Cabrera-Sanfeliix P, Arnau A, Darling GR, and Sanchez-Portal D.
Journal of Physical Chemistry B **110**, 48, 24559 (2006).

A TDDFT study of the excited states of DNA bases and their assemblies.

Varsano V, Di Felice R, Marqués MAL, and Rubio A.
Journal of Physical Chemistry B **110**, 7129 (2006).

Reaction mechanism of the acidic hydrolysis of highly twisted amides: rate acceleration caused by the twist of the amide bond.

Mujika JI, Formoso E, Mercero JM, and Lopez X.
Journal of Physical Chemistry B, **110**, 15000 (2006).

Modeling nanostructures with vicinal surfaces.

Mugarza A, Schiller F, Kuntze J, Cerdón J, Ruiz-Osés M, and Ortega JE.
Journal of Physics **C18**, S27 (2006).

Electron-phonon contribution to the phonon and excited electron (hole) linewidths in bulk Pd.

Sklyadneva IYu, Leonardo A, Echenique PM, Ereemeev SV, and Chulkov EV.
Journal of Physics: Condensed Matter **18**, 7923 (2006).

Mode coupling theory predictions for a limited valency attractive square well model.

Zaccarelli E, Saika-Voivod I, Moreno J, La Nave E, Buldyrev SV, Sciortino F,
and Tartaglia P.
Journal of Physics: Condensed Matter **18**, S2373 (2006).

On the affinity regulation of the metal ion dependent adhesion sites in integrins.

Zaccarelli E, Saika-Voivod I, Moreno J, La Nave E, Buldyrev SV, Sciortino F,
and Tartaglia P.
Journal of the American Chemical Society **128**, 3554 (2006).

Pressure Induced Metallization of Germane.

Martínez-Canales M, Bergara A, Feng J, and Grochala W.
Journal of Physics and Chemistry of Solids **67**, 2095 (2006).

Seeded growth of submicron Au colloids with quadrupole plasmon resonance modes.

Rodríguez-Fernández J, Pérez-Juste J, García de Abajo FJ, and Liz-Marzán L.
Langmuir **22**, 7007 (2006).

Quasielastic neutron scattering study on the effect of blending on the dynamics of head-to-head poly(propylene) and poly(ethylene-propylene).

Aparicio RP, Arbe A, Colmenero J, Frick B, Willner L, Richter D, and Fetters LJ. *Macromolecules* **39**, 1060 (2006).

On the Molecular Motions Originating from the Dielectric γ -Relaxation of Bisphenol-A Polycarbonate.

Alegria A, Mitxelena O, and Colmenero J. *Macromolecules* **39**, 2691 (2006).

Dynamic confinement effects in polymer blends. A quasielastic neutron scattering study of the dynamics of poly(ethylene oxide) in a blend with poly(vinyl acetate).

Tyagi M, Arbe A, Colmenero J, Frick B, and Stewart JR. *Macromolecules* **39**, 3007 (2006).

Pressure-temperature dependence of polymer segmental dynamics. Comparison between the Adam-Gibbs approach and density scalings.

Schwartz GA, Colmenero J, and Alegria A. *Macromolecules* **39**, 3931 (2006).

Local structure of syndiotactic poly(methyl methacrylate). A combined study by neutron diffraction with polarization analysis and atomistic molecular dynamics simulations.

Genix AC, Arbe A, Alvarez F, Colmenero J, Schweika W, and Richter D. *Macromolecules* **39**, 3947 (2006).

Modeling the dynamics of head-to-head polypropylene in blends with polyisobutylene.

Cangialosi D, Alegria A, and Colmenero J. *Macromolecules* **39**, 448 (2006).

Self- and collective dynamics of syndiotactic poly(methyl methacrylate). A combined study by quasielastic neutron scattering and atomistic molecular dynamics simulations.

Genix AC, Arbe A, Alvarez F, Colmenero J, Farago B, Wischnewski A, and Richter D. *Macromolecules* **39**, 6260 (2006).

Predicting the time scale of the component dynamics of miscible polymer blends: The polyisoprene/poly(vinylethylene) case.

Cangialosi D, Alegria A, and Colmenero J. *Macromolecules* **39**, 7149 (2006).

Probing the electronic properties of self-organized poly(3-dodecylthiophene) monolayer single chain scale.

Wirtz L, Marini A, Grüning M, and Rubio A. *Nano Letters* **6**, 1711 (2006).

Raman spectroscopy of Single-Wall boron nitride nanotubes.

Arenal R, Ferrari AC, Reich S, Wirtz L, Mevellec JY, Lefrant S, Rubio A, and Lois A. *Nano Letters* **6**, 1812 (2006).

Electronic excitation energies of ZnSi nanoparticles.

Matxain JM, Eriksson LA, Mercero JM, Ugalde JM, Spano E, Hamad S, and Catlow CRA. *Nanotechnology* **17**, 4100 (2006).

Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets.

Cabria I, López MJ, and Alonso JA. *Nanotechnology* **17**, 778 (2006).

Corrigendum: Complete photo-fragmentation of the deuterium molecule.

Weber T, Czausch AO, Jagutzki O, Müller AK, Mergel V, Kheifets A, Rotenberg E, Meigs G, Prior MH, Daveau S, Landers A, Cocke CL, Osipov T, Díez Muiño R, Schmidt-Böcking H, and Dörner R. *Nature* **443**, 1014 (2006).

Interacting Bose gases in quasi-one-dimensional optical lattices.

Cazalilla MA, Ho AF, and Giamarchi T. *New Journal of Physics* **8**, 158 (2006).

Curvature of the total electron density at critical coupling: attractive impurity in an electron gas.

Galindo A, Nagy I, Díez Muiño R, and Echenique PM. *New Journal of Physics* **8**, 299 (2006).

Strong coupling of light to flat metals via a buried nanovoid lattice: the interplay of localized and free plasmons.

Teperik TV, Popov VV, García de Abajo FJ, Abdelsalam P, Barlett N, Kelf TA, Suguwara Y, and Baumberg JJ. *Optic Express* **14**, 1965 (2006).

Spectroscopic study of Nd³⁺/Yb³⁺ in disordered potassium bismuth molybdate laser crystals.

Balda R, Fernández J, Iparraguirre I, and Al-Saleh M. *Optical Materials* **28**, 11, 1247 (2006).

Effect of concentration on the infrared emissions of Tm³⁺ ions in lead niobium germanate glasses.

Balda R, Fernandez J, Arriandiaga MA, Lacha LM, and Fernandez-Navarro JM. *Optical Materials* **28**, 11, 1253 (2006).

Mie plasmon enhanced diffraction of light from nanoporous metal surfaces.

Teperik TV, Popov VV, García de Abajo FJ, Kelf TA, Sugawara A, Baumberg JJ, Abdelsalam M, and Bartlett PN. *Optics Express* **14**, 11964-11971 (2006).

Extraordinary optical reflection from sub-wavelength cylinder arrays.

Gómez-Medina R, Laroche M, and Sáenz JJ. *Optics Express* **14**, 3730 (2006).

Infrared to visible upconversion of Nd³⁺ ions in KPb₂Br₅ low phonon crystal.

Balda R, Fernandez J, Nyein EE, Hommerich U.
Optics Express **14**, 3993 (2006).

Site and lattice resonances in metallic hole arrays.

García de Abajo FJ, Sáenz JJ, Campillo I, and Dolado JS.
Optics Express **14**, 7 (2006).

Plasmons in nearly touching metallic nanoparticles: singular response in the limit of touching dimers.

Romero I, Aizpurua J, Bryant GW, and García de Abajo FJ.
Optics Express **14**, 9988 (2006).

Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin polymerization.

Silanes I, Mercero JM, and Ugalde JM.
Organometallics **25**, 4483 (2006).

Effects of Mn clustering on ferromagnetism in (Ga,Mn)As.

Raebiger H, Hynninen T, Ayuela A, and Von Boehm J.
Physica B **376**, 643 (2006).

Octopus: a tool for the application of time-dependent density functional theory.

Castro A, Marques MAL, Appel H, Oliveira M, Rozzi CA, Andrade X, Lorenzen F, Gross EKV, and Rubio A.
Physica Status Solidi (b) **243**, 2465 (2006).

Buckling in boron sheets and nanotubes.

Cabria I, Alonso JA, and López MJ.
Physica Status Solidi **203**, 6, 1105 (2006).

Energy absorption of a Bose gas in a periodically modulated optical lattice.

Iucci A, Cazalilla MA, Ho AF and Giamarchi T.
Physical Review A (Rapid Communications) **73**, 041608 (2006).

Fermions in optical lattices near a Feshbach resonance: from band insulator to Mott insulator.

Ho AF.
Physical Review A (Rapid Communications) **73**, 061601 (2006).

Quantum-size effects in the energy loss of charged particles interacting with a confined two-dimensional electron gas.

Borisov AG, Juaristi JJ, Díez Muiño R, Sanchez-Portal D and Echenique PM.
Physical Review A **73**, 012901 (2006).

Photoelectron emission from metal surfaces by ultrashort laser pulses.

Faraggi MN, Gravielle MS, and Silkin VM.
Physical Review A **73**, 032901 (2006).

Exact non-Born-Oppenheimer wave functions for three-particle Hookean systems with arbitrary masses.

Lopez X, Ugalde JM, Echevarría L, and Ludeña EV.
Physical Review A **74**, 042504 (2006).

Effect of spatial nonlocality on the density functional band gap.

Grüning M, Marini A, and Rubio A.
Physical Review B (rapid communications) **74**, 161103 (2006).

Lifetimes of the image-state resonances at metal surfaces.

Borisov AG, Chulkov EV and Echenique PM.
Physical Review B **73**, 073402 (2006).

Lifetimes and inelastic mean free path of low-energy excited electrons in Fe, Ni, Pt, and Au: Ab initio GW+T calculations.

Zhukov VP, Chulkov EV, and Echenique PM.
Physical Review B **73**, 125105 (2006).

Multiple electron-hole scattering effects on quasiparticle properties in homogeneous electron gas.

Nechaev IA and Chulkov EV.
Physical Review B **73**, 165112 (2006).

An exact Coulomb cutoff technique for supercell calculations.

Rozzi CA, VarsanoD, Marini A, Gross EKV, and Rubio A.
Physical Review B **73**, 205119 (2006).

Experimental time-resolved photoemission and ab initio study of lifetimes of excited electrons in Mo and Rh.

Mönnich A, Lange J, Bauer M, Aeschlimann M, Nechaev IA, Zhukov VP, Echenique PM, and Chulkov EV.
Physical Review B **74**, 035102 (2006).

Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: detailed support for nonempirical density functionals.

Pitarke JM, Constantin L, and Perdew JP.
Physical Review B **74**, 045121 (2006).

Numerical study of bound states for point charges shielded by the response of a homogeneous two-dimensional electron gas.

Nagy I, Puska MJ, and Zabala N.
Physical Review B **74**, 115411 (2006).

Vibrations insubmonolayer structures of Na on Cu (111).

Borisova SD, Rusina GG, Ereemeev SV, Benedek G, Echenique PM, Sklyadneva IYu, and Chulkov EV.
Physical Review B **74**, 165412 (2006).

Complexity and Fermi surface deformation in compressed lithium.

Rodríguez-Prieto A, Bergara A, Silkin VM, and Echenique PM.
Physical Review B **74**, 172104 (2006).

- Superexchange coupling in iron/silicon layered structures.
Tugushev VV, Menshov VN, Nechaev IA, and Chulkov EV.
Physical Review B **74**, 184423 (2006).
- Strain effects on the electronic structure of strongly coupled self-assembled InAs/GaAs quantum dots: Tight-binding approach.
Jaskólski W, Zielinski M, Bryant GW, and Aizpurua J.
Physical Review B **74**, 195339 (2006).
- Spin-resolved two-photon photoemission study of the surface resonance state on Co/Cu (001).
Andreyev O, Koroteev YuM, Sánchez-Albaneda M, Cinchetti M, Bihlmayer G, Chulkov EV, Lange J, Steeb F, Bauer M, Echenique PM, Blügel S, and Aeschlimann M.
Physical Review B **74**, 195416 (2006)
- Structural determination of the Bi(110) a low-energy diffraction and ab-initio calculations:
Sun J, Mikkelsen A, Fuglsang Jensen M, Koroteev YM, Bihlmayer G, Chulkov EV, Adams DL, Hofmann Ph, and Pohl K.
Physical Review B **74**, 245406 (2006).
- Surface electronic structures of La(0001) and Lu(0001).
Wegner D, Bauer A, Koroteev YM, Bihlmayer G, Chulkov EV, Echenique PM, and Kaindl G.
Physical Review B **73**, 115403 (2006).
- Anomalous dynamic arrest in a mixture of large and small particles.
Moreno AJ, and Colmenero J.
Physical Review E **74**, 021409 (2006).
- Electrons and hydrogen-bond connectivity in liquid water.
Fernandez-Serra MV and Artacho E.
Physical Review Letters **96**, 016404 (2006).
- Structures and potential superconductivity in SiH₄ at high pressure: en route to metallic hydrogen.
Feng J, Grochala W, Jaroń T, Hoffmann R, Bergara A, and Ashcroft NW.
Physical Review Letters **96**, 017006 (2006).
- Excitons in boron nitride nanotubes: dimensionality effects.
Wirtz L, Marini A, and Rubio A.
Physical Review Letters **96**, 126104 (2006).
- First-principle description of correlation effects in layered materials.
Marini A, García-González P, and Rubio A.
Physical Review Letters **96**, 136404 (2006).
- Reply to the comment on "Fermi gap stabilization of an incommensurate two-dimensional superstructure".
Schiller F, Cerdón J, Vyalikh D, Rubio A, and Ortega JE.
Physical Review Letters **96**, 29702 (2006).
- Asymptotics of the dispersion interaction: analytic benchmarks for van derWaals energy functionals.
Dobson JF, White A, and Rubio A.
Physical Review Letters **96**, 73201 (2006).
- Anti-Stokes laser cooling in bulk erbium-doped materials - art. no. 033001
Fernandez J, Garcia-Adeva AJ, Balda R.
Physical Review Letters **97**, 033001 (2006).
- Why N₂ molecules with thermal energy abundantly dissociate on W(100) and not on W(110).
Alducin M, Díez Muño R, Busnengo HF, and Salin A.
Physical Review Letters **97**, 056102 (2006).
- Infrared imaging of single nanoparticles via strong field enhancement in a scanning nanogap.
Cvitkovic A, Ocelic N, Aizpurua J, Guckenberger R, and Hillenbrand R.
Physical Review Letters **97**, 060801 (2006).
- Dissipation-driven quantum phase transitions in a Tomonaga-Luttinger liquid electrostatically coupled to a metallic gate.
Cazalilla MA, Sols F, and Guinea F.
Physical Review Letters **97**, 076401 (2006).
- Extreme ultrafast dynamics of quasiparticles excited in surface electronic bands.
Lazic P, Silkin VM, Chulkov EV, Echenique PM, and Gumhalter B.
Physical Review Letters **97**, 086801 (2006).
- Real-time Ab initio simulations of excited carrier dynamics in carbon nanotubes
Yamamoto, Y, Rubio A, and Tománek D.
Physical Review Letters **97**, 126104 (2006).
- Role of spin-orbit coupling and hybridization effects in the electronic structure of ultrathin Bi films.
Hirahara T, Nagao T, Matsuda I, Bihlmayer G, Chulkov EV, Koroteev YM, Echenique PM, Saito M and Hasegawa S.
Physical Review Letters **97**, 146803 (2006).
- Effect of suddenly turning on interactions in the luttinger model.
Cazalilla, MA.
Physical Review Letters **97**, 156403 (2006).
- Comment on "pressure dependence of fragile-to-strong transition and a possible second critical point in supercooled confined water".
Cerveny S, Colmenero J, and Alegria A.
Physical Review Letters **97**, 189802 (2006).
- Homogeneous Fermi liquid with "artificial" repulsive inverse square law interparticle potential energy
Nagy I, March NH, Echenique PM.
Physics and Chemistry of Liquids **44**, 571 (2006).

Electronic kinetic energy decrease as two metallic parallel C nanotubes are brought together from infinity.

March N and Rubio A.
Physics Letters A 358, 334 (2006).

Ab initio study of the double row model of the Si(553)-Au reconstruction.

Riikonen S, and Sanchez-Portal D.
Surface Science 600, 1201 (2006).

Scattering of Cu(100) image state electrons from single Cu adatoms and vacancies: A comparative study.

Olsson FE, Borisov AG, and Gauyacq JP.
Surface Science 600, 2184 (2006).

Electron-phonon interaction in a free standing beryllium monolayer.

Leonardo A, Sklyadneva IYu, Echenique PM and Chulkov EV.
Surface Science 600, 3715 (2006).

Electron-phonon interaction and hole (electron) lifetimes on Be(0001).

Sklyadneva IY, Chulkov EV, Echenique PM, and Eiguren A.
Surface Science 600, 3792 (2006).

Decay of electronic excitations in bulk metals and at surfaces.

Chulkov EV, Leonardo A, Nechaev IA, and Silkin VM.
Surface Science 600, 3795 (2006).

X-ray photoelectron diffraction study of Cu(111): Multiple scattering investigation.

Despont L, Naumovic D, Clerc F, Koitzsch C, Garnier MG, García de Abajo FJ, Van Hove MA and Aebi P.
Surface Science 600, 380 (2006).

Metal-insulator transition in the In/Si(111) surface.

Riikonen, S, Ayuela A, and Sanchez-Portal D.
Surface Science 600, 3821 (2006).

Dynamical response function of a compressed lithium monolayer.

Rodriguez-Prieto A, Silkin VM, Bergara A, and Echenique PM.
Surface Science 600, 3856 (2006).

Charge-density oscillations at (111) noble metal surfaces.

Silkin VM, Nechaev IA, Chulkov EV, and Echenique PM.
Surface Science 600, 3875 (2006).

The Rashba-effect at metallic surfaces.

Bihlmayer G, Koroteev YM, Echenique PM, Chulkov EV, and Blugel S.
Surface Science 600, 3888 (2006).

Vibrations on Al surfaces covered by sodium.

Rusina GG, Ereemeev SV, Borisova SD, Sklyadneva Yu, and Chulkov EV.
Surface Science 600, 3921 (2006).

Methylthiolate adsorption on Au(111): Energetics, vibrational modes and STM imaging.

Gonzalez-Lakunza N, Lorente N, and Arnau A.
Surface Science 600, 4039 (2006).

Surface electronic structure of $O(2 \times 1)/Cu(110)$: Role of the surface state at the zone boundary Y-point in STS.

Corriol A, Hager J, Matzdorf R, Arnau A.
Surface Science 600, 4310 (2006).

Non-Gaussian energy landscape of a simple model for strong network-forming liquids: Accurate evaluation of the configurational entropy.

Moreno AJ, Saika-Voivod I, Zaccarelli E, La Nave E, Buldyrev SV, Tartaglia P, and Sciortino F.
The Journal of Chemical Physics 124, 204509 (2006).

A thermodynamic approach to the fragility of glass-forming polymers.

Cangialosi D, Alegría A, and Colmenero J.
The Journal of Chemical Physics 124, 024906 (2006).

Gel to glass transition in simulation of a valence-limited colloidal system.

Zaccarelli E, Saika-Voivod I, Buldyrev SV, Moreno AJ, Tartaglia P, and Sciortino F.
The Journal of Chemical Physics 124, 124908 (2006).

Electronic structure and excitations of oligoacenes from ab initio calculations.

Kadantsev ES, Stott MJ, and Rubio A.
The Journal of Chemical Physics 124, 134901 (2006).

Density functionals from many-body perturbation theory: the bandgap for semiconductors and insulators.

Grüning M, Marini A, and Rubio A.
The Journal of Chemical Physics 124, 154108 (2006).

Describing the component dynamics in miscible polymer blends: Towards a fully predictive model.

Schwartz GA, Cangialosi D, Alegría A, and Colmenero J.
The Journal of Chemical Physics 124, 154904 (2006).

Is there a higher-order mode coupling transition in polymer blends?

Moreno AJ and Colmenero J.
The Journal of Chemical Physics 124, 184906 (2006).

Water dynamics in n-propylene glycol aqueous solutions.

Cervený S, Schwartz GA, Alegría A, Bergman R, and Swenson J.
The Journal of Chemical Physics 124, 194501 (2006).

Electron correlation in the $3^1\Sigma_g^+$ and $2^1\Sigma_u^+$ excited states lithium molecule.

Wang J, Zhang L, Wang Y, and Ugalde JM.
The Journal of Chemical Physics 125, 234102 (2006).

- Logarithmic relaxation in a kinetically constrained model.
Moreno AJ and Colmenero J.
The Journal of Chemical Physics **125**, 016101 (2006).
- Photoabsorption spectra of Ti8C12 metalcarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory.
Martinez JI, Castro A, Rubio A, and Alonso JA.
The Journal of Chemical Physics **125**, 074311 (2006).
- Low sticking probability in the nonactivated dissociation of N2 molecules on W (110).
Alducin M, Díez Muiño R, Busnengo HF, and Salin A.
The Journal of Chemical Physics **125**, 144705 (2006).
- Electronic structure of C-60 on Au(887).
Schiller F, Ruiz-Oses M, Ortega JE Segovia P, Martínez-Blanco J, Doyle BP, Pérez-Dieste V, Lobo J, Neel N, Berndt R, and Kroger J.
The Journal of Chemical Physics **125**, 144719 (2006).
- Plasticizer effect on the dynamics of polyvinylchloride studied by dielectric spectroscopy and quasielastic neutron scattering.
Zorn R, Monkenbusch M, Richter D, Alegria A, Colmenero J, and Farago B.
The Journal of Chemical Physics **125**, 154904 (2006).
- Relaxation scenarios in a mixture of large and small spheres: dependence on the size disparity.
Moreno AJ and Colmenero J.
The Journal of Chemical Physics **125**, 164507 (2006).
- Influence of plasmon-assisted charge exchange processes on ion-induced electron emission from metals.
Rösler M, Pauly N, Dubus A, Díez Muiño R, and Alducin M.
Vacuum **80**, 554 (2006).
- Energy and lifetime of surface plasmon from first-principles calculations
Silkin VM and Chulkov EV.
Vacuum **81**, 186 (2006).

- Dynamics of electrons and holes at surfaces.
Chulkov EV, Leonardo A, Sklyadneva IYu, and Silkin VM.
Applied Surface Science **254**, 383 (2007).
- Monolayer adsorption of water on NaCl(1 0 0).
Cabrera-Sanfelix P, Holloway S, and Darling GR.
Applied Surface Science **254**, 87 (2007).
- Protein Side Chains that Facilitate Mg/Al Exchange in Model Protein Binding Sites.
Rezabal E, Mercero JM, Lopez X and Ugalde JM.
ChemPhysChem **8**, 2119 (2007).
- Endohedral Stannaspherenes Mn@Sn12 and its Dimer: Ferromagnetic or Antiferromagnetic?
Matxain JM, Piris M, Formoso E, Mercero JM, Lopez X, and Ugalde JM.
ChemPhysChem Communications **8**, 2096 (2007).
- Electron correlation in the GK state of the hydrogen molecule.
Wang J, Wang Y, Shengliang Lv, and Ugalde JM.
Chemical Physics **127**, 074307 (2007).
- Ab initio study of 2,3,7,8-tetrachlorinated dibenzo-p-dioxin adsorption on single wall carbon nanotubes.
Solange B, Fagan, EJG, Santos AG, Souza Filhob J, Mendes Filho and Fazzio A.
Chemical Physics Letters **437**, 79 (2007).
- Spectroscopic fingerprints of amine and imide functional groups in self-assembled monolayers.
Ruiz-Oses M, González-Lakunza N, Silanes I, Gourdon A, Arnau A, and Ortega JE.
ChemPhysChem **8**, 1722 (2007).
- Dynamics of confined water in different environments.
Cervený S, Colmenero J, Alegria A.
European Physical Journal **141**, 49 (2007).
- Theoretical study of molecular hydrogen clusters. Growth models and magic numbers.
Martínez JI, Isla M. and Alonso JA.
European Physical Journal D **43**, 61 (2007).
- Complexation of AlIII by Aromatic Amino Acids in the Gas Phase.
Rezabal E, Marino T, Mercero JM, Russo N, Ugalde JM.
Inorganic Chemistry **46**, 6413 (2007).
- Valence electron correlation energy embracing the diamond-lattice materials C through Sn.
March NH and Rubio A.
International Journal Materials Science Simulations **1**, 16 (2007).

Metal Ion Dependent Adhesion Sites in Integrins: A Combined DFT and QMC Study on Mn²⁺.

San Sebastian E, Matxain JM, Eriksson LA, Stote RH, Dejaegere A, Cossio FP, and Lopez X.
The Journal of Physical Chemistry B **111**, 9099 (2007).

Experimental time-resolved photoemission and ab initio GW + T study of lifetimes of excited electrons in ytterbium.

Marienfeld A, Cinchetti M, Bauer M, Aeschlimann M, Zhukov VP, Chulkov EV, and Echenique PM.
Journal of Physics: Condensed Matter **19**, 496213 (2007).

Assessment of approximate density functional methods for the study of the interactions of Al(III) with aromatic amino acids.

Rezabal R, Marino T, Mercero JM, Russo N, and Ugalde JM.
Journal Chemical Theory and Computational **3**, 1830 (2007).

Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities.

Andrade X, Botti S, Marques MAL and Rubio A.
Journal of Chemical Physics **126**, 184106 (2007).

“Self-concentration” effects on the dynamics of a polychlorinated biphenyl diluted in 1,4-polybutadiene.

Cangialosi D, Alegría A, and Colmenero J.
Journal of Chemical Physics **126**, 204904 (2007).

On the structure of the first hydration layer on NaCl: 100Role of hydrogen bonding.

Cabrera-Sanfelix P, Arnau A, Darling GR, and Sanchez-Portal D.
Journal of Chemical Physics **126**, 214707 (2007).

Nonequilibrium GW approach to quantum transport in nano-scale contacts.

Thygesen KS and Rubio A.
Journal of Chemical Physics **126**, 91101 (2007).

Silicate chain formation in the nanostructure of cement-based materials.

Ayuela A, Dolado JS, Campillo I, de Miguel YR, Erkizia E, Sánchez-Portal D, Rubio A, Porro A, and Echenique PM.
Journal of Chemical Physics **127**, 164710 (2007).

Homogeneous line width of rare-earth-doped glasses for levels in a Stark level ladder: A new simple rule.

Auzel F, Balda R, and Fernández J.
Journal of Luminiscence **122**, 453 (2007).

Combined electrochromic and plasmonic optical responses in conducting polymer/metal nanoparticle films.

Pacios R, Marcilla R, Pozo-Gonzalo C, Pomposo JA, Grande H, Aizpurua J, and Mecerreyes D.
Journal of Nanoscience and Nanotechnology **7**, 2938 (2007).

Laser action and upconversion of Nd³⁺ in tellurite bulk glass.

Iparraguirre I, Azkargorta J, Fernández-Navarro JM, Al-Saleh M, Fernández J, and Balda R.
Journal of Non-Crystalline Solids **353**, 990 (2007).

Phonons in ordered c (2 x 2) phases of Na and Li on Al (001).

Rusina GG, Eremeev SV, Borisova SD, Sklyadneva IYu, Echenique PM, and Chulkov EV.
Journal of Physics: Condensed Matter **19**, 266005 (2007).

Transport mean-free-path in K5Bi1-xNdx (MoO4)4 laser crystal powders.

Illarramendi MA, Aramburu I, Fernández J, Balda R, and Al-Saleh M.
Journal of Physics: Condensed Matter **19**, 036206 (2007).

Plasmon excitation in beryllium: inelastic X-ray scattering experiments and first-principles calculations.

Tirao G, Stutz G, Silkin VM, Chulkov EV, and Cusatis C.
Journal of Physics: Condensed Matter **19**, 046297 (2007).

Spectroscopy and frequency upconversion in Nd³⁺-doped TeO₂-TiO₂-Nb₂O₅ glass.

Balda R, Fernández J, Arriandiaga MA, Fdez-Navarro JM.
Journal of Physics: Condensed Matter **19**, 086223 (2007).

Atomic Motions in the alpha/beta-Region of Glass-Forming Polymers. Molecular versus Mode Coupling Theory Approach.

Colmenero J, Narros A, Alvarez F, Arbe A, Moreno AJ.
Journal of Physics: Condensed Matter **19**, 205127 (2007).

Anomalous Relaxation in Binary Mixtures: A Dynamic Facilitation Picture.

Moreno AJ, and Colmenero J.
Journal of Physics: Condensed Matter **19**, 205144 (2007).

Tests of mode coupling theory in a simple model for two-component miscible polymer blends.

Moreno AJ, and Colmenero J.
Journal of Physics: Condensed Matter **19**, 466112 (2007).

Characterization of light scattering in translucent ceramics.

Illarramendi MA, Aramburu I, Fernández J, Balda R, Williams SN, Adegoké JA and Noginov MA.
Journal of the Optical Society of America B-Optical Physics **24**, 43 (2007).

New Solids Based on B12N12 Fullerenes.

Matxain JM, Eriksson LA, Mercero JM, Lopez X, Piris M, Ugalde JM, Poater J, Matito E, and Sola M.
Journal Physical Chemistry C **111**, 13354 (2007).

Nanohole plasmons in optically thin gold films.

Rindzevicius T, Alaverdyan Y, Sepulveda B, Pakizeh T, Kall M, Hillenbrand R, Aizpurua J, and García de Abajo FJ.
Journal Physical Chemistry C **111**, 1207 (2007).

- Chemisorption of Sulfur and Sulfur-Based Simple Molecules on Au(111).
Gonzalez-Lakunza N, Lorente N, and Arnau A.
Journal Physical Chemistry C **111**, 12383 (2007).
- Spontaneous emergence of Cl-anions from NaCl(100) at low relative humidity.
Cabrera-Sanfeliu P, Sanchez-Portal D, Verdaguier A, Darling GR, Salmeron M,
and Arnau A.
Journal Physical Chemistry C **111**, 8000 (2007).
- Dissociative Adsorption of Water at Vacancy Defects in Graphite.
Cabrera-Sanfeliu P and Darling GR.
The Journal of Physical Chemistry C **111**, 18258 (2007).
- Global search in photoelectron diffraction structure determination using genetic algorithms.
Viana ML, Díez Muiño R, Soares EA, Van Hove MA, and de Carvalho VE.
Journal of Physics: Condensed Matter **19**, 446002 (2007).
- Single Component Dynamics in Miscible Poly(vinyl methyl ether)/Polystyrene Blends under Hydrostatic Pressure.
Schwartz GA, Colmenero J, and Alegría A.
Macromolecules **40**, 3246 (2007).
- Dynamic confinement effects in polymer blends. A quasielastic neutron scattering study of the slow component in the blend poly(vinyl acetate)/poly(ethylene oxide).
Tyagi M, Arbe A, Alegría A, Colmenero J, and Frick B.
Macromolecules **40**, 4568 (2007).
- Low-energy acoustic plasmons at metal surfaces.
Diaconescu B, Pohl K, Vattuone L, Savio L, Hofmann P, Silkin VM, Pitarke JM, Chulkov EV, Echenique PM, Fariás D, and Rocca M.
Nature **448** (7149), 57 (2007).
- Attosecond spectroscopy in condensed matter.
Cavalleri AL, Muller N, Uphues Th, Yakovlev V, Baltuska A, Horvath B, Schmidt B, Blümel L, Holzwarth R, Hendel S, Drescher M, Kleineberg U, Echenique PM, Kienberger R, Krausz F and Heinzmann U.
Nature **449**, (7165) 1029 (2007).
- Surface patterning: Self-assembly works for superlattices.
Ortega JE and de Abajo FJG.
Nature Nanotechnology **2**, 601 Oct (2007).
- Spin dependent screening and Auger neutralization of singly-charged noble gas ions in metals.
Juaristi JI and Alducin M.
Nuclear Instruments and Methods in Physics Research B **256**, 24 (2007).
- Two dimensional behaviour of friction at a metal surface with a surface state.
Alducin M, Silkin VM and Juaristi JI.
Nuclear Instruments and Methods in Physics Research B **256**, 383 (2007).
- Spin-dependent electron excitation and emission in the neutralization of He⁺ ions at paramagnetic surfaces.
Alducin M and Rösler M.
Nuclear Instruments and Methods in Physics Research B **256**, 423 (2007).
- Stopping power of a degenerate electron gas for slow ions: Role of relative kinematics in Z1-oscillation below the Fermi velocity.
Vincent R and Nagy I.
Nuclear Instruments and Methods in Physics Research B **258**, 182 (2007).
- Dynamic screening and electron dynamics in low-dimensional metal systems.
Silkin VM, Quijada M, Vergniory MG, Alducin M, Borisov AG, Díez Muiño R, Juaristi JI, Sánchez-Portal D, Chulkov EV, and Echenique PM.
Nuclear Instruments and Methods in Physics Research B **258**, 72 (2007).
- Z1 oscillations in the spin polarization of electrons excited by slow ions in a spin-polarized electron gas.
Vincent R, Juaristi JI, and Nagy I.
Nuclear Instruments and Methods in Physics Research B **258**, 79 (2007).
- First luminescence study of the new oxyborate Na₃La₉O₃(BO₃)₈:Nd³⁺.
Balda R, Jubera V, Frayret C, Pechev S, Olazcuaga R, Gravereau P, Chaminade JP, Al-Saleh M, and Fernández J.
Optical Materials **30**, 122 (2007).
- Characterization of light propagation in Nd_xY_{1-x}Al(BO₃)₄ laser crystal powders.
Illarramendi MA, Cascales C, Aramburu I, Balda R, Orera VM, and Fernández J.
Optical Materials **30**, 126 (2007).
- Spectroscopy and concentration quenching of the infrared emissions in Tm³⁺-doped TeO₂-TiO₂-Nb₂O₅ glass.
Balda R, Fernández J, García Revilla S, and Fdez-Navarro JM.
Optics Express **15**, 6750 (2007).
- Absorption of BN nanotubes under the influence of a perpendicular electric field.
Attacalite C, Wirtz L, Marini A, and Rubio A.
Physica Status Solidi **244**, 4288 (2007).
- Mechanical properties of cementitious crystalline calcium-silicate-hydrates: comparison with C-S-H gels.
Manzano H, Dolado JS, Guerrero A, and Ayuela A.
Physica Status Solidi A **204**, 1775 (2007).
- Diffusion and Relaxation Dynamics in Cluster Crystals.
Moreno AJ and Likos CN.
Physical Review Letters **99**, 107801 (2007).
- Size effects in angle-resolved photoelectron spectroscopy of free rare-gas clusters.
Rolles D, Zhang H, Peñic ZD, Bilodeau RC, Wills A, Kukk E, Rude BS, Ackerman GD, Bozek JD, Díez Muiño R, García de Abajo FJ, and Berrah N.
Physical Review A **75**, 031201 (2007).

Time-dependent density-functional calculation of the stopping power for protons and antiprotons in metals.

Quijada M, Borisov AG, Nagy I, Díez Muiño R, and Echenique PM.
Physical Review A **75**, 042902 (2007).

Competition between vortex unbinding and tunneling in an optical lattice.

Cazalilla MA, Lucci A, and Giamarchi T.
Physical Review A **75**, 051603(R) (2007).

Electron emission and energy loss in grazing collisions of protons with insulator surfaces.

Gravielle MS, Aldazabal I, Arnau A, Ponce VH, Miraglia JE, Aumayr F, Lederer S, and Winter H.
Physical Review A **76**, 012904 (2007).

3d-shell contribution to the energy loss of protons during grazing scattering from Cu(111) surfaces.

Gravielle MS, Alducin M, Juaristi JI, and Silkin VM.
Physical Review A **76**, 044901 (2007).

Momentum density and spatial form of correlated density matrix in model two-electron atoms with harmonic confinement.

Akbari A, March NH, and Rubio A.
Physical Review A **76**, 32510 (2007).

Adsorption and electronic excitation of biphenyl on Si(100): a theoretical STM analysis.

Dubois M, Delerue C, and Rubio A.
Physical Review B (Rapid Communications) **75**, 41302 (2007).

Determination of Compton profiles at solid surfaces from first-principles calculations.

Lemell C, Arnau A, and Burgdörfer J.
Physical Review B **75**, 014303 (2007).

Quantum well states in ultrathin Bi films: Angle-resolved photoemission spectroscopy and first-principles calculations study.

Hirahara T, Nagao T, Matsuda I, Bihlmayer G, Chulkov EV, Koroteev YuM, and Hasegawa S.
Physical Review B **75**, 035422 (2007).

Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids.

Pemmaraju CD, Archer T, Sánchez-Portal D, and Sanvito S.
Physical Review B **75**, 045101 (2007).

Role of surface states in Auger neutralization of He⁺ ions on Ag surfaces.

Sarasola A, Silkin VM, and Arnau A.
Physical Review B **75**, 045104 (2007).

Band mapping in the one-step photoemission theory: Multi-Bloch-wave structure of final states and interference effects.

Krasovskii EE, Strocov VN, Barrett N, Berger H, Schattke W, and Claessen R.
Physical Review B **75**, 045432 (2007).

Microscopic investigation of laser induced structural changes in single-wall carbon nanotubes.

Jeschke HO, Romero AH, García ME, and Rubio A.
Physical Review B **75**, 125112 (2007).

Restored quantum size effects of Pb overlayers at high coverages.

Ayuela A, Ogando E, and Zabala N.
Physical Review B **75**, 153403 (2007).

Thermally induced defects and the lifetime of electronic surface states.

Fuglsang Jensen M, Kim TK, Bengio S, Sklyadneva IYu, Leonardo A, Ereemeev SV, Chulkov EV, and Hofmann Ph.
Physical Review B **75**, 153404 (2007).

Quantum Monte Carlo modelling of the spherically averaged structure factor of a many-electron system.

Gaudoin R and Pitarke JM.
Physical Review B **75**, 155105 (2007).

Role of the electric field in surface electron dynamics above the vacuum level.

Pascual JI, Corriol C, Ceballos G, Aldazabal I, Rust H-P, Horn K, Pitarke JM, Echenique PM, and Arnau A.
Physical Review B **75**, 165326 (2007).

Surface-plasmon polaritons in a lattice of metal cylinders.

Pitarke JM, Inglesfield JE, and Giannakis N.
Physical Review B **75**, 165415 (2007).

Excited states of Na nanoislands on the Cu(111) surface.

Hakala T, Puska MJ, Borisov AG, Silkin VM, Zabala N, and Chulkov EV.
Physical Review B **75**, 165419 (2007).

Strong variation of dielectric response and optical properties of lithium under pressure.

Silkin VM, Rodriguez-Prieto A, Bergara A, Chulkov EV, and Echenique PM.
Physical Review B **75**, 172102 (2007).

Enhanced Rashba spin-orbit splitting in Bi/Ag(111) and Pb/Ag(111) surface alloys.

Bihlmayer G, Blügel S, and Chulkov EV.
Physical Review B **75**, 195414 (2007).

Electron-electron interaction in a two-dimensional electron gas: Bound states at low densities.

Nagy I, Puska MJ, and Zabala N.
Physical Review B **75**, 233105 (2007).

Decay and dephasing of image-state electrons induced by Cs adsorbates on Cu(100) at intermediate coverage.

Kazansky AK, Silkin VM, Chulkov EV, Borisov AG, and Gauyacq JP.
Physical Review B **75**, 235412 (2007).

Ab initio calculation of the phonon-induced contribution to the electron-state linewidth on the Mg(0001) surface versus bulk Mg.

Leonardo A, Sklyadneva IY, Silkin VM, Echenique PM, and Chulkov EV.
Physical Review B 76, 035404 (2007).

Interplay between the electronic and the atomic structure in the Si(557)-Au reconstruction from first principles.

Riikonen S and Sanchez-Portal D.
Physical Review B 76, 035410 (2007).

Ultrafast dynamics and decoherence of quasiparticles excited in surface bands: Preasymptotic decay and dephasing of quasiparticles states.

Lazic P, Silkin VM, Chulkov EV, Echenique PM, and Gumhalter B.
Physical Review B 76, 045420 (2007).

Crystal structure of SiH4 at high pressure.

Degtyareva O, Martínez Canales A, Bergara A, Chen X-J, Song Y, Struzhkin VV, Mao H-k, and Hemley RJ.
Physical Review B 76, 064123 (2007).

Strength of dipolar backflow patterns around slow protons in three and two dimensional electron gases.

Vincent R, Nagy I, and Zaremba E.
Physical Review B 76, 073301 (2007).

Second harmonic generation from arrays of subwavelength cylinders.

Marinica DC, Borisov AG, and Shabanov SV.
Physical Review B 76, 085311 (2007).

Image potential states of supported metallic nanoslands.

Borisov AG, Hakala T, Puska MJ, Silkin VM, Zabala N, Chulkov EV, and Echenique PM.
Physical Review B 76, 121402 (2007).

Direct observation of spin splitting in bismuth surface states.

Hirahara, T, Miyamoto K, Matsuda I, Kadono T, Kimura A, Nagao T, Bihlmayer G, Chulkov EV, Qiao S, Shimada K, Namatame H, Taniguchi M, and Hasegawa S.
Physical Review B 76, 153305 (2007).

Two-dimensional localization of fast electrons in p (2x2) - Cs/Cu (111).

Chis V, Caravati S, Butti G, Trioni MI, Cabrera-Sanfelix P, Arnau A, and Hellsing B.
Physical Review B 76, 153404 (2007).

Excited electron dynamics in bulk ytterbium: Time-resolved two-photon photoemission and GW + T ab initio calculations.

Zhukov VP, Chulkov EV, Echenique PM, Marienfeld A, Bauer M, and Aeschlimann M.
Physical Review B 76, 193107 (2007).

Theoretical study of the photoabsorption spectrum of small chromium clusters.

Martínez JI and Alonso JA.
Physical Review B 76, 205409 (2007).

Water adsorption on O(2x2)/Ru (0001): STM experiments and first-principles calculations.

Cabrera-Sanfelix P, Sánchez-Portal D, Mugarza A, Shimizu TM, Salmeron M, and Arnau A.
Physical Review B 76, 205438 (2007).

Influence of hydrogen absorption on low-energy electronic collective excitations in palladium.

Silkin VM, Chernov IP, Echenique PM, Koroteev YuM, and Chulkov EV.
Physical Review B 76, 245105 (2007).

GW-lifetimes of quasiparticle excitations in paramagnetic transition metals.

Nechaev IA, Chulkov EV, and Echenique PM.
Physical Review B 76, 245125 (2007).

Phenylene ring dynamics in phenoxy and the effect of intramolecular linkages on the dynamics of some engineering thermoplastics below the glass transition temperature.

Arrese-Igor S, Arbe A, Alegría A, Colmenero J, and Frick B.
Physical Review E 75, 051801 (2007).

Route to calculate the length scale for the glass transition in polymers.

Cangialosi D, Alegría A, and Colmenero J.
Physical Review E 75, 011514 (2007).

Broadband dielectric study of oligomer of poly(vinyl acetate): A detailed comparison of dynamics with its polymer analog.

Tyagi M, Alegría A, and Colmenero J.
Physical Review E 75, 061805 (2007).

Positron-annihilation-lifetime response and broadband dielectric relaxation spectroscopy: Diethyl phthalate.

Bartos J, Alegría A, Sausa O, Tyagi M, Gómez D, Kristiak J, and Colmenero J.
Physical Review E 76, 031503 (2007).

Positron-annihilation-lifetime response and broadband dielectric relaxation spectroscopy: Diethyl phthalate.

Bartos J, Alegría A, Sausa O, Tyagi M, Gómez D, Kristiak J, and Colmenero J.
Physical Review E 76, 031503 (2007).

Optimal control of quantum rings by terahertz laser pulses.

Räsänen E, Castro A, Werschnik J, Rubio A, and Gross EKU.
Physical Review Letters 98, 157404 (2007).

Polymer Chain Dynamics in a Random Environment: Heterogeneous Mobilities.

Niedzwiedz K, Wischniewski A, Monkenbusch M, Richter D, Genix AC, Arbe A, Colmenero J, Strauch M, and Straube E.
Physical Review Letters 98, 168301 (2007).

Determination of the hole lifetime from photoemission: Ti 3d States in TiTe2.

Krasovskii EE, Rossnagel K, Fedorov A, Schattke W, and Kipp L.
Physical Review Letters 98, 217604 (2007).

Vibrational properties of hexagonal boron nitride: inelastic X-ray scattering and ab initio calculations.

Serrano J, Bosak A, Arenal R, Krisch M, Watanabe K, Taniguchi T, Kanda H, Rubio A, and Wirtz L.
Physical Review Letters **98**, 95503 (2007).

Hellman-Feynman operator sampling in diffusion Monte Carlo calculations.

Gaudoin R and Pitarke JM.
Physical Review Letters **99**, 126406 (2007).

Sublattice magnetizations in non-zero magnetic field in an antiferromagnetic infinite-range Ising model.

Ayuela A, Kleinb DJ, and March NH.
Physics Letters A **362**, 468 (2007).

Exact correlated kinetic energy related to the electron density for two-electron model atoms with harmonic confinement.

March NH, Akbari A, and Rubio A.
Physics Letters A **370**, 509 (2007).

Ab-initio calculation of quasiparticle excitations lifetime in transition metals using GW approximation.

Nechaev IA, Zhukov VP, and Chulkov EV.
Physics of Solid State **49**, 1811 (2007).

Exchange-correlation effects in ab-initio calculations of plasmon dispersion and width in metals.

Nechaev IA, Silkin VM, and Chulkov EV.
Physics of Solid State **49**, 1820 (2007).

Dynamics of surface-localised electronic excitations studied with the scanning tunnelling microscope.

Kröger J, Becker M, Jensen H, von Hofe Th, Néel N, Limot L, Berndt R, Crampin S, Pehlke E, Corriol C, Silkin VM, Sanchez-Portal D, Arnau A, Chulkov EV, and Echenique PM.
Progress in Surface Science **82**, 293 (2007).

Slab calculations and Green function recursive methods combined to study the electronic structure of surfaces: application to Cu(111)-(4x4)-Na.

Sanchez-Portal D.
Progress in Surface Science **82**, 313 (2007).

Band structure effects in the surface plasmon at the Be(0001) surface.

Silkin VM, Chulkov EV, and Echenique PM.
Radiation effects and defects in solid **162**, 483 (2007).

Interaction of slow multicharged ions with surfaces.

Lemell C, Alducin M, Burgdörfer J, Juaristi JI, Schiessl K, Solleder B, and Tökesi K.
Radiation Physics and Chemistry **76**, 412 (2007).

Theory of surface plasmons and surface-plasmon polaritons.

Pitarke JM, Silkin VM, Chulkov EV, and Echenique PM.
Reports on Progress Physics **70**, 1 (2007).

The simplest double slit: interference and entanglement in double photoionization of H₂.

Akoury D, Kreidi K, Jahnke T, Weber Th, Staudte A, Schöffler M, Neumann M, Titze J, Ph. H. Schmidt L, Czasch A, Jagutzki O, Costa Fraga RA, Grisenti RE, Díez Muiño R, Cherepkov NA, Semenov SK, Ranitovic P, Cocke CL, Osipov T, Adaniya H, Thompson JC, Prior MH, Belkacem A, Landers A, Schmidt- Böcking H, and Dörner R.
Science **318**, 949 (2007).

Spin polarization of electrons emitted in the neutralization of He⁺ ions in solids.

Alducin M, Juaristi JI, Díez Muiño R, Roesler M, and Echenique PM.
Springer Tracts in Modern Physics **225**, 153 (2007).

Diffusion properties of Cu(001) - c(2x2)-Pd surface alloys.

Eremeev SV, Rusina GG, and Chulkov EV.
Surface Science **601**, 3640 (2007).

Dissociative adsorption of N₂ on W(110): Theoretical study of the dependence on the incidence angle.

Alducin M, Díez Muiño R, Busnengo HF, and Salin A.
Surface Science **601**, 3726 (2007).

Electron-phonon interaction in magnesium: From the monolayer to the Mg (0001) surface.

Leonardo A, Yu Sklyadneva I, Echenique PM, and Chulkov EV.
Surface Science **601**, 4018 (2007).

Electron-phonon contribution to hole linewidth of the surface state on Al(001).

Yu Sklyadneva I, Leonardo A, Echenique PM, and Chulkov EV.
Surface Science **601**, 4022 (2007).

Role of final states in photoemission from Al(111).

Krasovskii EE, Schattke W, Jiricek P, Dudr V, and Bartos I.
Surface Science **601**, 4105 (2007).

Dynamic screening and electron-electron scattering in low-dimensional metallic systems.

Silkin VM, Quijada M, Díez Muiño R, Chulkov EV, and Echenique PM.
Surface Science **601**, 4546 (2007).

Electron-phonon coupling in a sodium monolayer on Cu(111).

Eremeev SV, Yu. Sklyadneva I, Echenique PM, Borisova SD, Benedek G, Rusina GG, and Chulkov EV.
Surface Science **601**, 4553 (2007).

Ultrafast charge transfer and atomic orbital polarization.

Deppe M, Föhlich A, Hennies F, Nagasono M, Beye M, Sanchez-Portal D, Echenique PM, and Wurth W.
Journal of Chemical Physics **127**, 174708 (2007).

On the formation of cementitious C-S-H nanoparticles.

Manzano H, Ayuela A, and Dolado JS.
Journal of Computer-Aided Materials Design **14**, 45 (2007).

Long-range van derWaals interactions in density functional theory.

Alonso JA and Mañanes A.
Theoretical Chemistry Accounts **117**, 467 (2007).

Self-assembly of silicide quantum dot arrays on stepped silicon surfaces by reactive epitaxy.

Fernández L, Löffler M, Cordon J, and Ortega JE.
Applied Physics Letters **91**, 263106 (2007).

Quantum size effects of Pb overlayers at high coverages.

Ayuela A, Ogando E, and Zabala N.
Applied Surface Science **254**, 29 (2007).

Adam-Gibbs based model to describe the single component dynamics in miscible polymer blends under hydrostatic pressure.

Schwartz GA, Alegria A, Colmenero J.
Journal of Chemical Physics **127**, 154907 (2007).

Dielectric properties of water in amorphous mixtures of polymers and other glass forming materials.

Cervený S, Colmenero J, and Alegria A
Journal of Non-Crystalline Solids **353**, 4523 (2007).

An attosecond time-resolved study of strong-field atomic photoionization.

Kazansky AK and Kabachnik NM.
Journal of Physics B: Atomic, Molecular and Optical Physics **40**, 299 (2007).

Interaction of the charged deuterium cluster D_3^+ with femtosecond laser pulses.

Isla M, and Alonso JA.
Journal Physical Chemistry C **111**, 17765 (2007).

Nesting Induced Peierls-type Instability for Compressed Li-cl16.

Rodríguez-Prieto A, Silkin VM and Bergara A.
Journal Physical Society Japan **76**, 21 (2007).

Metal-Organic Honeycomb Nanomeshes with Tunable Cavity Size.

Schlickum U, Decker R, Klappenberger F, Zoppellaro G, Klyatskaya S, Ruben M, Silanes I, Arnau A, Kern K, Brune H and Jarth JV.
Nano Letters **7**, 12, 3813 (2007).

Low energy quasiparticle dispersion of graphite by angle-resolved photoemission spectroscopy.

Grüneis A, Pichler T, Shiozawa H, Attacalite C, Wirtz L, Molodtsov SL, Follath R, Weber R and Rubio A.
Physica Status Solidi **244**, 4129 (2007).

Simple dynamic exchange-correlation kernel of a uniform electron gas.

Constantin L and Pitarke, JM.
Physical Review B **75**, 245127 (2007).

Including the probe tip in theoretical models of inelastic scanning tunneling spectroscopy: CO on Cu(100).

Teobaldi G, Peñalba M, Arnau A, Lorente N, and Hofer WA.
Physical Review B **76**, 235407 (2007).

Self-energy and lifetime of Shockley and image states on Cu(100) and Cu(111): Beyond the GW approximation of many-body theory.

Vergniory MG, Pitarke JM, and Echenique PM.
Physical Review B **76**, 245416 (2007).

First-principles calculation of charge transfer at surfaces: The case of core-excited Ar^* ($2p_{3/2}^3 4s$) on Ru(0001).

Sanchez-Portal D, Menzel D, and Echenique PM.
Physical Review B **76**, 235406 (2007).

Electronic stopping power in LiF from first principles.

Pruneda JM, Sanchez-Portal D, Arnau A, Juaristi JI, and Artacho E.
Physical Review Letters **99**, 235501 (2007).

Dielectric secondary relaxation and phenylene ring dynamics in bisphenol-A polycarbonate.

Alegria A, Arrese-Igor S, Mitxelena O, and Colmenero J.
Journal of Non Crystalline Solids **353**, 4262 (2007).

Dielectric study of the segmental relaxation of low and high molecular weight polystyrenes under hydrostatic pressure.

Schwartz GA, Colmenero J, and Alegria A.
Journal of Non Crystalline Solids **353**, 4298 (2007).

On the momentum transfer dependence of the atomic motions in the α -relaxation range.

Polymers vs. low molecular weight glass-forming systems.

Sacristán J, Alvarez F, and Colmenero J.
Europhysics Letters **80**, 38001 (2007).

Segmental dynamics in miscible polymer blends: recent results and open questions. (Review by invitation.)

Colmenero J, and Arbe A.
Soft Matter **3**, 1474 (2007).

Light propagation in optical crystal powders: effects of particle size and volume filling factor.

García-Ramiro B, Illarramendi MA, Aramburu I, Fernández J, Balda R, and Al-Saleh M.
Journal of Physics Condensed Matter **19**, 456213 (2007).