



INSTITUT DE CIÈNCIA DE  
MATERIALS DE BARCELONA



# ARTICLES IN JOURNALS

A large, abstract graphic composed of overlapping, semi-transparent geometric shapes in shades of blue and grey, creating a sense of depth and movement.

2017



**CSIC**

CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

# ARTICLES IN JOURNALS 2017

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ICMAB's researchers published 201 articles in international scientific journals in 2017. In this report you can find them ordered by research lines and ranked according their Impact Factor. Twenty-seven of them belong to two sublines and are repeated in each one.

<b>RL1 - ENERGY STORAGE AND CONVERSION.....</b>	<b>3</b>
<b>RL2 - SUPERCONDUCTORS FOR POWER APPLICATIONS.....</b>	<b>14</b>
<b>RL3 - OXIDE ELECTRONICS.....</b>	<b>17</b>
<b>RL4 - MOLECULAR ELECTRONICS.....</b>	<b>24</b>
<b>RL5 - MULTIFUNCTIONAL NANOSTRUCTURED BIOMATERIALS.....</b>	<b>31</b>

# Articles in Journals 2017

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## RL1 - ENERGY STORAGE AND CONVERSION

1. Hussain, H.; Tocci, G.; Woolcot, T.; Torrelles, X.; Pang, C. L.; Humphrey, D. S.; Yim, C. M.; Grinter, D. C.; Cabailh, G.; Bikondoa, O.; Lindsay, R.; Zegenhagen, J.; Michaelides, A.; Thornton, G.  
**Structure of a model TiO<sub>2</sub> photocatalytic interface**  
(2017), *Nature Materials*, 16 (4), pp. 461-+
2. Tang, Zheng; Ma, Zaifei; Sanchez-Diaz, Antonio; Ullbrich, Sascha; Liu, Yuan; Siegmund, Bernhard; Mischok, Andreas; Leo, Karl; Campoy-Quiles, Mariano; Li, Weiwei; Vandewal, Koen  
**Polymer: Fullerene Bimolecular Crystals for Near-Infrared Spectroscopic Photodetectors**  
(2017), *Advanced Materials*, 29 (33), 1702184
3. Cartoixa, Xavier; Palummo, Maurizia; Hauge, Hakon Ikaros T.; Bakkers, Erik P. A. M.; Rurali, Riccardo  
**Optical Emission in Hexagonal SiGe Nanowires**  
(2017), *Nano Letters*, 17 (8), pp. 4753-4758
4. Landa-Medrano, Imanol; Sorrentino, Andrea; Stievano, Lorenzo; Ruiz de Larramendi, Idoia; Pereiro, Eva; Lezama, Luis; Rojo, Teofilo; Tonti, Dino  
**Architecture of Na-O<sub>2</sub> battery deposits revealed by transmission X-ray microscopy**  
(2017), *Nano Energy*, 37, pp. 224-231
5. Graczykowski, B.; El Sachat, A.; Reparaz, J. S.; Sledzinska, M.; Wagner, M. R.; Chavez-Angel, E.; Wu, Y.; Volz, S.; Wu, Y.; Alzina, F.; Sotomayor Torres, C. M.  
**Thermal conductivity and air-mediated losses in periodic porous silicon membranes at high temperatures**  
(2017), *Nature Communications*, 8, 415
6. Collado, Laura; Jansson, Ingrid; Platero-Prats, Ana E.; Perez-Dieste, Virginia; Escudero, Carlos; Molins, Elies; Casas i Doucastela, Lluís; Sanchez, Benigno; Coronado, Juan M.; Serrano, David P.; Suarez, Silvia; de la Pena-O'Shea, Victor A.  
**Elucidating the Photoredox Nature of Isolated Iron Active Sites on MCM-41**  
(2017), *ACS Catalysis*, 7 (3), pp. 1646-1654

7. Guzzetta, Fabrizio; Roig, Anna; Julian-Lopez, Beatriz  
**Ultrafast Synthesis and Coating of High-Quality  $\beta$ -NaYF<sub>4</sub>:Yb<sup>3+</sup>,Ln<sup>3+</sup> Short Nanorods**  
(2017), *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*, 8 (23), pp. 5730-5735  
*Also included in RL5*
8. Kiefer, David; Yu, Liyang; Fransson, Erik; Gomez, Andres; Primetzhofer, Daniel; Amassian, Aram; Campoy-Quiles, Mariano; Muller, Christian  
**A Solution-Doped Polymer Semiconductor: Insulator Blend for Thermoelectrics**  
(2017), *Advanced Science*, 4 (1), 1600203
9. Aramberri, H; Muñoz, M.C; Cerdá, J.I.  
**A realistic topological p–n junction at the Bi<sub>2</sub>Se<sub>3</sub> (0001) surface based on planar twin boundary defects**  
(2017), *Nano Research*, 10 (5), pp. 1784-1793
10. Silva-Guillen, J. A.; Canadell, E.; Ordejon, P.; Guinea, F.; Roldan, R.  
**Anisotropic features in the electronic structure of the two-dimensional transition metal trichalcogenide TiS<sub>3</sub>: electron doping and plasmons**  
(2017), *2D Materials*, 4 (2), 25085  
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11. Isacson, Andreas; Cummings, Aron W.; Colombo, Luciano; Colombo, Luigi; Kinaret, Jari M.; Roche, Stephan  
**Scaling properties of polycrystalline graphene: a review**  
(2017), *2D Materials*, 4 (1), 12002  
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12. Dorling, Bernhard; Sanchez-Diaz, Antonio; Arteaga, Oriol; Veciana, Andrea; Isabel Alonso, Maria; Campoy-Quiles, Mariano  
**Controlled Pinning of Conjugated Polymer Spherulites and Its Application in Detectors**  
(2017), *Advanced Optical Materials*, 5 (19), 1700276
13. Pinto, Alexandre; Griera, Rosa; Molins, Elies; Fernandez, Israel; Bosch, Joan; Amat, Mercedes  
**Access to Enantiopure 5-, 7-, and 5,7-Substituted *cis*-Decahydroquinolines: Enantioselective Synthesis of (-)-Cermizine B**  
(2017), *Organic Letters*, 19 (7), pp. 1714-1717
14. Perez, Maria; Ramos, Carlos; Massi, Lucia; Gazzola, Silvia; Taglienti, Chiara; Yayik, Nihan; Molins, Elies; Viayna, Antonio; Javier Luque, F.; Bosch, Joan; Amat, Mercedes  
**Enantioselective Synthesis of Spiro[indolizidine-1,3'-oxindoles]**  
(2017), *Organic Letters*, 19 (15), pp. 4050-4053

15. Olivares-Marin, Mara; Sorrentino, Andrea; Pereiro, Eva; Tonti, Dino  
**Discharge products of ionic liquid-based Li-O<sub>2</sub> batteries observed by energy dependent soft x-ray transmission microscopy**  
(2017), *Journal of Power Sources*, 359, pp. 234-241
16. Cuxart, M. G.; Sics, I.; Goni, A. R.; Pach, E.; Sauthier, G.; Paradinas, M.; Foerster, M.; Aballe, L.; Moreno Fernandez, H.; Carlino, V.; Pellegrin, E.  
**Inductively coupled remote plasma-enhanced chemical vapor deposition (rPE-CVD) as a versatile route for the deposition of graphene micro- and nanostructures**  
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17. Palomino, Pablo; Suarez-Guevara, Jullieth; Olivares-Marin, Mara; Ruiz, Vanesa; Dubal, Deepak P.; Gomez-Romero, Pedro; Tonti, Dino; Enciso, Eduardo  
**Influence of texture in hybrid carbon-phosphomolybdic acid materials on their performance as electrodes in supercapacitors**  
(2017), *Carbon*, 111, pp. 74-82
18. Terron, Angel; Moreno-Vachiano, Blas; Bauza, Antonio; Garcia-Raso, Angel; Fiol, Juan Jesus; Barcelo-Oliver, Miquel; Molins, Elies; Frontera, Antonio  
**X-ray Crystal Structure of a Metalled Double-Helix Generated by Infinite and Consecutive C\*-Ag<sup>I</sup>-C\* (C\*: N<sup>1</sup>-Hexylcytosine) Base Pairs through Argentophilic and Hydrogen Bond Interactions**  
(2017), *Chemistry-A European Journal*, 23 (9), pp. 2103-2108
19. Ferrer, Ingrid; Fontrodona, Xavier; Roig, Anna; Rodriguez, Montserrat; Romero, Isabel  
**A Recoverable Ruthenium Aqua Complex Supported on Silica Particles: An Efficient Epoxidation Catalyst**  
(2017), *Chemistry-A European Journal*, 23 (17), pp. 4096-4107
20. Rodriguez-Martinez, Xabier; Vezie, Michelle S.; Shi, Xingyuan; McCulloch, Iain; Nelson, Jenny; Goni, Alejandro R.; Campoy-Quiles, Mariano  
**Quantifying local thickness and composition in thin films of organic photovoltaic blends by Raman scattering**  
(2017), *Journal of Materials Chemistry C*, 5 (29), pp. 7270-7282
21. Oleshkevich, Elena; Vinas, Clara; Romero, Isabel; Choquesillo-Lazarte, Duane; Haukka, Matti; Teixidor, Francesc  
**m-Carboranylphosphinate as Versatile Building Blocks To Design all Inorganic Coordination Polymers**  
(2017), *Inorganic Chemistry*, 56 (10), pp. 5502-5505  
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22. Cuesta, Ana; Ichikawa, Rodrigo U.; Londono-Zuluaga, Diana; De la Torre, Angeles G.; Santacruz, Isabel; Turrillas, Xavier; Aranda, Miguel A. G.  
**Aluminum hydroxide gel characterization within a calcium acuminate cement paste by combined Pair Distribution Function and Rietveld analyses**  
(2017), *Cement and Concrete Research*, 96, pp. 1-12
23. Antidormi, Aleandro; Melis, Claudio; Canadell, Enric; Colombo, Luciano  
**Assessing the Performance of Eumelanin/Si Interface for Photovoltaic Applications**  
(2017), *Journal of Physical Chemistry C*, 121 (21), pp. 11576-11584  
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24. Landa-Medrano, Imanol; Olivares-Marin, Mara; Bergner, Benjamin; Pinedo, Ricardo; Sorrentino, Andrea; Pereiro, Eva; Ruiz de Larramendi, Idoia; Janek, Jurgen; Rojo, Teofilo; Tonti, Dino  
**Potassium Salts as Electrolyte Additives in Lithium-Oxygen Batteries**  
(2017), *Journal of Physical Chemistry C*, 121 (7), pp. 3822-3829
25. Royo, Miguel; Antidormi, Aleandro; Rurali, Riccardo  
**A Thermal Switch for Coherent Phonons Based on a Molecular Junction**  
(2017), *Journal of Physical Chemistry C*, 121 (19), pp. 10571-10576
26. Lopez-Dominguez, Pedro; Lopez-Periago, Ana M.; Fernandez-Porras, Francisco J.; Fraile, Julio; Tobias, Gerard; Domingo, Concepcion  
**Supercritical CO<sub>2</sub> for the synthesis of nanometric ZIF-8 and loading with hyperbranched aminopolymers. Applications in CO<sub>2</sub> capture**  
(2017), *Journal Of CO2 Utilization*, 18, pp. 147-155
27. Fuentes, Isabel; Andrio, Andreu; Teixidor, Francesc; Vinas, Clara; Compan, Vicente  
**Enhanced conductivity of sodium versus lithium salts measured by impedance spectroscopy. Sodium cobaltacarboranes as electrolytes of choice**  
(2017), *Physical Chemistry Chemical Physics*, 19 (23), pp. 15177-15186
28. Verrelli, R.; Arroyo-de-Dompablo, M. E.; Tchitchekova, D.; Black, A. P.; Frontera, C.; Fuertes, A.; Palacin, M. R.  
**On the viability of Mg extraction in MgMoN<sub>2</sub>: a combined experimental and theoretical approach**  
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29. Tsang, Min Ying; Rodriguez-Hermida, Sabina; Stylianou, Kyriakos C.; Tan, Fangchang; Negi, Divya; Teixidor, Francesc; Vinas, Clara; Choquesillo-Lazarte, Duane; Verdugo-Escamilla, Cristobal; Guerrero, Miguel; Sort, Jordi; Juanhuix, Jordi; MasPOCH, Daniel; P  
**Carborane Bis-pyridylalcohols as Linkers for Coordination Polymers: Synthesis, Crystal Structures, and Guest-Framework Dependent Mechanical Properties**  
(2017), *Crystal Growth & Design*, 17 (2), pp. 846-857
30. Lopez-Periago, Ana M.; Portoles-Gil, Nuria; Lopez-Dominguez, Pedro; Fraile, Julio; Saurina, Javier; Aliaga-Alcalde, Nuria; Tobias, Gerard; Ayllon, Jose A.; Domingo, Concepcion  
**Metal-Organic Frameworks Precipitated by Reactive Crystallization in Supercritical CO<sub>2</sub>**  
(2017), *Crystal Growth & Design*, 17 (5), pp. 2864-2872
31. Bueyuekyazi, Mehtap; Fischer, Thomas; Yu, Penmgei; Coll, Mariona; Mathur, Sanjay  
**A cobalt(II) heteroarylalkenolate precursor for homogeneous Co<sub>3</sub>O<sub>4</sub> coatings by atomic layer deposition**  
(2017), *Dalton Transactions*, 46 (38), pp. 12996-13001  
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32. Casan-Pastor, Nieves; Rius, Jordi; Vallcorba, Oriol; Peral, Inma; Oro-Sole, Judith; Cook, Daniel S.; Walton, Richard I.; Garcia, Alberto; Munoz-Rojas, David  
**Ag<sub>2</sub>Cu<sub>3</sub>Cr<sub>2</sub>O<sub>8</sub>(OH)<sub>4</sub>: a new bidimensional silver-copper mixed-oxyhydroxide with in-plane ferromagnetic coupling**  
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33. Papior, Nick; Lorente, Nicolas; Frederiksen, Thomas; Garcia, Alberto; Brandbyge, Mads  
**Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA**  
(2017), *Computer Physics Communications*, 212, pp. 8-24  
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34. Antonio Seijas-Bellido, Juan; Escorihuela-Sayalero, Carlos; Royo, Miquel; Ljungberg, Mathias P.; Wojdel, Jacek C.; Iniguez, Jorge; Rurali, Riccardo  
**A phononic switch based on ferroelectric domain walls**  
(2017), *Physical Review B*, 96 (14), 140101  
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35. Caddeo, Claudia; Melis, Claudio; Ronchi, Andrea; Giannetti, Claudio; Ferrini, Gabriele; Rurali, Riccardo; Colombo, Luciano; Banfi, Francesco  
**Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach**  
(2017), *Physical Review B*, 95 (8), 85306
36. Treacy, Jon P. W.; Hussain, Hadeel; Torrelles, Xavier; Grinter, David C.; Cabailh, Gregory; Bikondoa, Oier; Nicklin, Christopher; Selcuk, Sencer; Selloni, Annabella; Lindsay, Robert; Thornton, Geoff  
**Geometric structure of anatase TiO<sub>2</sub>(101)**  
(2017), *Physical Review B*, 95 (7), 75416
37. Aramberri, Hugo; Rurali, Riccardo; Iniguez, Jorge  
**Thermal conductivity changes across a structural phase transition: The case of high-pressure silica**  
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38. Terron, Angel; Tomas, Llorenç; Bauza, Antonio; Garcia-Raso, Angel; Fiol, Juan J.; Molins, Elies; Frontera, Antonio  
**The first X-ray structure of a silver-nucleotide complex: interaction of ion Ag(I) with cytidine-5'-monophosphate**  
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39. Portoles-Gil, Nuria; Parra-Aliana, Ricard; Alvarez-Larena, Angel; Domingo, Concepcion; Ayllon, Jose A.; Lopez-Periago, Ana  
**Bottom-up approach for the preparation of hybrid nanosheets based on coordination polymers made of metal-diethylxaloacetate complexes linked by 4,4'-bipyridine**  
(2017), *Crystengcomm*, 19 (34), pp. 4972-4982  
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40. Perez del Pino, A.; Gyorgy, E.; Alshaikh, I.; Pantoja-Suarez, F.; Andujar, J. L.; Pascual, E.; Amade, R.; Bertran-Serra, E.  
**Laser-driven coating of vertically aligned carbon nanotubes with manganese oxide from metal organic precursors for energy storage**  
(2017), *Nanotechnology*, 28 (39), 395405
41. El Sachat, A.; Reparaz, J. S.; Spiece, J.; Alonso, M., I; Goni, A. R.; Garriga, M.; Vaccaro, P. O.; Wagner, M. R.; Kolosov, O., V; Sotomayor Torres, C. M.; Alzina, F.  
**Thermal transport in epitaxial Si<sub>1-x</sub>Gex alloy nanowires with varying composition and morphology**  
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42. Raya-Moreno, Marti; Aramberri, Hugo; Antonio Seijas-Bellido, Juan; Cartoixa, Xavier; Rurali, Riccardo  
**Thermal conductivity of hexagonal Si and hexagonal Si nanowires from first-principles**  
(2017), *Applied Physics Letters*, 111 (3), 32107
43. Bejaoui, A.; Alonso, M. I.; Garriga, M.; Campoy-Quiles, M.; Goni, A. R.; Hetsch, F.; Kershaw, S. V.; Rogach, A. L.; To, C. H.; Foo, Y.; Zapien, J. A.  
**Evaluation of the dielectric function of colloidal Cd<sub>1-x</sub>Hg<sub>x</sub>Te quantum dot films by spectroscopic ellipsometry**  
(2017), *Applied Surface Science*, 421, pp. 295-300
44. Alonso, M. I.; Funke, S.; Gonzalez, A.; Garriga, M.; Vaccaro, P. O.; Goni, A. R.; Ruiz, A.; Alonso, M.; Thiesen, P. H.  
**Spectroscopic imaging ellipsometry of self-assembled SiGe/Si nanostructures**  
(2017), *Applied Surface Science*, 421, pp. 547-552
45. Tchitchekova, D. S.; Monti, D.; Johansson, P.; Barde, F.; Randon-Vitanova, A.; Palacin, M. R.; Ponrouch, A.  
**On the Reliability of Half-Cell Tests for Monovalent (Li<sup>+</sup>, Na<sup>+</sup>) and Divalent (Mg<sup>2+</sup>, Ca<sup>2+</sup>) Cation Based Batteries**  
(2017), *Journal of the Electrochemical Society*, 164 (7), pp. A1384-A1392
46. Rius, Jordi; Vallcorba, Oriol; Crespi, Anna; Colombo, Fernando  
**Increasing data completeness in synchrotron tts-microdiffraction experiments for delta-recycling phasing of low-symmetry compounds**  
(2017), *Zeitschrift fur Kristallographie-Crystalline Materials*, 232 (12), pp. 827-834
47. Barrena, Esther; Buss, Felix; Perez-Rodriguez, Ana; Sanyal, Monamie; Schmidt-Hansberg, Benjamin; Klein, Michael F. G.; Scharfer, Philip; Schabel, Wilhelm; Lemmer, Uli  
**In situ Studies of Morphology Formation in Solution-Processed Polymer-Fullerene Blends**  
(2017), *Elementary Processes in Organic Photovoltaics*, 272, pp. 1-24
48. Stankiewicz, Jolanta; Torrelles, Xavier; Luis Garcia-Munoz, Jose; Blasco, Javier  
**Structural and electrical properties of indium oxide thin films grown by pulsed laser deposition in oxygen ambient**  
(2017), *Journal of Alloys and Compounds*, 694, pp. 1280-1286  
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49. Queralto, Albert; Perez del Pino, Angel; Logofatu, Constantin; Datcu, Angela; Amade, Roger; Alshaiikh, I.; Bertran, Enric; Urzica, Iuliana; Gyorgy, Eniko  
**MAPLE synthesis of reduced graphene oxide/silver nanocomposite electrodes: Influence of target composition and gas ambience**  
(2017), *Journal of Alloys and Compounds*, 726, pp. 1003-1013
50. Camps, I.; Borlaf, M.; Colomer, M. T.; Moreno, R.; Duta, L.; Nita, C.; Perez del Pino, A.; Logofatu, C.; Serna, R.; Gyorgy, E.  
**Structure-property relationships for Eu doped TiO<sub>2</sub> thin films grown by a laser assisted technique from colloidal sols**  
(2017), *RSC Advances*, 7 (60), pp. 37643-37653
51. Kepic, Dejan; Sandoval, Stefania; Perez del Pino, Angel; Gyorgy, Eniko; Cabana, Laura; Ballesteros, Belen; Tobias, Gerard  
**Nanosecond Laser-Assisted Nitrogen Doping of Graphene Oxide Dispersions**  
(2017), *Chemphyschem*, 18 (8), pp. 935-941
52. Estarellas, Carolina; Arioli, Federica; Perez, Maria; Are, Celeste; Hevia, David; Molins, Elies; Javier Luque, F.; Bosch, Joan; Amat, Mercedes  
**Origin of the Base-Dependent Facial Selectivity in Annulation Reactions of Nazarov-Type Reagents with Unsaturated Indolo[2,3- $\alpha$ ] quinolizidine Lactams**  
(2017), *European Journal of Organic Chemistry*, 0 (27), pp. 3969-3979
53. Berencen, Y.; Mundet, B.; Rodriguez, J. A.; Montserrat, J.; Dominguez, C.; Garrido, B.  
**Hot electron engineering for boosting electroluminescence efficiencies of silicon-rich nitride light emitting devices**  
(2017), *Journal of Luminescence*, 183, pp. 26-31
54. Livneh, Tsachi; Reparaz, Juan S.; Goni, Alejandro R.  
**Low-temperature resonant Raman asymmetry in 2H-MoS<sub>2</sub> under high pressure**  
(2017), *Journal of Physics-Condensed Matter*, 29 (43), 435702
55. Colodrero, Rosario M. P.; Salcedo, Ines R.; Bazaga-Garcia, Montse; Milla-Perez, Diego F.; Duran-Martin, Jonatan D.; Losilla, Enrique R.; Moreno-Real, Laureano; Rius, Jordi; Aranda, Miguel A. G.; Demadis, Konstantinos D.; Olivera-Pastor, Pascual; Cabeza, A  
**Structural variability in M<sup>2+</sup> 2-hydroxy-phosphonoacetate moderate proton conductors**  
(2017), *Pure and Applied Chemistry*, 89 (1), pp. 75-87

56. Romero, Beatriz; del Pozo, Gonzalo; Arredondo, Belen; Martin-Martin, Diego; Gordo, Maria P. Ruiz; Pickering, Andrew; Perez-Rodriguez, Ana; Barrena, Esther; Garcia-Sanchez, Francisco J.  
**S-Shaped I-V Characteristics of Organic Solar Cells: Solving Mazhari's Lumped-Parameter Equivalent Circuit Model**  
(2017), *IEEE Transactions on Electron Devices*, 64 (11), pp. 4622-4627
57. Perez del Pino, Angel; Gyorgy, Eniko; Hussain, Shahzad; Luis Andujar, Jose; Pascual, Esther; Amade, Roger; Bertran, Enric  
**Laser-induced nanostructuring of vertically aligned carbon nanotubes coated with nickel oxide nanoparticles**  
(2017), *Journal of Materials Science*, 52 (7), pp. 4002-4015
58. Royo, Miquel; De Luca, Marta; Rurali, Riccardo; Zardo, Ilaria  
**A review on III-V core-multishell nanowires: growth, properties, and applications**  
(2017), *Journal of Physics D-Applied Physics*, 50 (14), 143001
59. Antidormi, Alejandro; Royo, Miquel; Rurali, Riccardo  
**Electron and phonon transport in twisted graphene nanoribbons**  
(2017), *Journal of Physics D-Applied Physics*, 50 (23), 234005
60. Ying Tsang, Min; Vinas, Clara; Teixidor, Francesc; Choquesillo-Lazarte, Duane; Giner Planas, Jose  
**Crystalline Inclusion Compounds of a Palladacyclic Tetraol Host Featuring o-Carborane Units**  
(2017), *European Journal of Inorganic Chemistry*, 0 (38-39), pp. 4589-4598  
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61. Doerling, Bernhard; Sandoval, Stefania; Kankla, Pacharapon; Fuertes, Amparo; Tobias, Gerard; Campoy-Quiles, Mariano  
**Exploring different doping mechanisms in thermoelectric polymer/carbon nanotube composites**  
(2017), *Synthetic Metals*, 225, pp. 70-75
62. Aiglsperger, Thomas; Proenza, Joaquin A.; Gali, Salvador; Rius, Jordi; Longo, Francisco; Domenech, Cristina  
**The supergene origin of ruthenian hexaferrum in Ni-laterites**  
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**Towards the synthesis of poly(azafulleroid)s: main chain fullerene oligomers for organic photovoltaic devices**  
(2017), *Polymer International*, 66 (10), pp. 1364-1371
64. Afkhami, Farhad Akbari; Khandar, Ali Akbar; Mahmoudi, Ghodrat; Amini, Mojtaba; Molins, Elies; Garczarek, Piotr; Lipkowski, Janusz; White, Jonathan M.; Kirillov, Alexander M.  
**New cadmium(II) and zinc(II) coordination polymers derived from a pyridine-hydrazone block: Self-assembly generation, structural and topological features, and theoretical analysis**  
(2017), *Inorganica Chimica Acta*, 458, pp. 68-76
65. Arrue, Lily; Rey, Marina; Rubilar-Hernandez, Carlos; Correa, Sebastian; Molins, Elies; Norambuena, Lorena; Zarate, Ximena; Schott, Eduardo  
**Synthesis, characterization, spectroscopic properties and DFT study of a new pyridazinone family**  
(2017), *Journal of Molecular Structure*, 1148, pp. 162-169
66. Vallcorba, Oriol; Casas, Lluís; Colomboa, Fernando; Frontera, Carlos; Rius, Jordi  
**First terrestrial occurrence of the complex phosphate chladniite: crystal-structure refinement by synchrotron through-the-substrate microdiffraction**  
(2017), *European Journal of Mineralogy*, 29 (2), pp. 287-293
67. Colombo, Fernando; Mugnaioli, Enrico; Vallcorba, Oriol; Garcia, Alberto; Goni, Alejandro R.; Rius, Jordi  
**Crystal structure determination of karibibite, an Fe<sup>3+</sup> arsenite, using electron diffraction tomography**  
(2017), *Mineralogical Magazine*, 81 (5), pp. 1191-1202  
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**X-ray diffraction and relativistic DFT studies on the molecular biomarker fac-Re(CO)<sub>3</sub>(4,4'-dimethyl-2,2'-bpy)(E-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol)(PF<sub>6</sub>)**  
(2017), *Chemical Papers*, 71 (10), pp. 2011-2022

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**Inclusion of [H<sub>3</sub>PW<sub>12</sub>O<sub>40</sub>] and [H<sub>4</sub>SiW<sub>12</sub>O<sub>40</sub>] into a Silica Gel Matrix via Sol-Gel Methodology**  
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(2017), *MRS Advances*, 2 (12), 1700163
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**Band Engineering of Dangling-Bond Wires on the Si(100)H Surface**  
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