



RESUMEN DE LA ACTIVIDAD INVESTIGADORA DEL DEPARTAMENTO DE SISTEMAS FÍSICOS, QUÍMICOS Y NATURALES. CURSO 2022/2023

- . Libros (0)
- . Capítulos de libros (10)
- . Artículos (97)
 - . Organización conferencias, cursos, jornadas y seminarios (3)
 - . Proyectos (24)
 - . Contratos (12)
 - . Estancias (0)
 - . Premios, cátedras, patentes (2)

LISTA DE ARTÍCULOS PUBLICADOS:

Área de Cristalografía y Mineralogía

- Moreno, M., Ortiz, R., & Ortiz, P. (2022). Remote sensing to assess the risk for cultural heritage: forecasting potential collapses due to rainfall in historic fortifications. International Journal of Building Pathology and Adaptation, (ahead-of-print).
- Moreno, M., Ortiz, R., & Ortiz, P. (2022). Review of satellite resources to assess environmental threats in rammed earth fortifications. Ge-conservacion, 21(1), 309-328.
- Moreno, M., Bertolín, C., Ortiz, P., & Ortiz, R. (2022). Satellite product to map drought and extreme precipitation trend in Andalusia, Spain: A novel method to assess heritage landscapes at risk. International Journal of Applied Earth Observation and Geoinformation, 110, 102810.
- Diaz, G. A., Ortiz, R., Moreno, M., & Ortiz, P. (2022). Vulnerability Assessment of Historic Villages in the Amazonas Region (Peru). International Journal of Architectural Heritage, 1-21.
- Maripaz Mateo; Javier Becerra; Ana Paula Zaderenko; Pilar Ortiz; Ginés Nicolás. Assessment by laser-induced breakdown spectroscopy of penetration depth in limestones of four nano-biocides



based on silver/titanium nanoparticles. Journal of Cultural Heritage this link is disabled. 58, pp. 237 - 244. 31/10/2022. ISSN 1296-2074. DOI: 10.1016/j.culher.2022.10.010

Área de Ecología

- David de la Lama-Calvente; María José Fernández-Rodríguez; Jacinto Gandullo; Irene Desena; Clara de la Osa; Ana Belén Feria; 2Antonia Jiménez- Rodríguez & Rafael Borja. Valorization of different landrace and commercial sorghum (*Sorghum bicolor* (L.) Moench) straw varieties by anaerobic digestion. *GCB Bioenergy* (00):1–14 (2022) DOI: 10.1111/gcbb.13025
- Delgado Baquerizo, M., Hu, H.-W., Maestre, F.T., Guerra, C.A., Eisenhauer, N., Eldridge, D.J., Zhu, Y.-G., Chen, Q.-L., Trivedi, P., Du, S., Makhalanyane, T.P., Verma, J.P., Gozalo, B., Ochoa, V., Asensio, S., Wang, L., Zaady, E., Illán, J.G., Siebe, C., Grebenc, T., Zhou, X., Liu, Y.-R., Bamigboye, A.R., Blanco-Pastor, J.L., Duran, J., Rodríguez, A., Mamet, S., Alfaro, F., Abades, S., Teixido, A.L., Peñaloza-Bojacá, G.F., Molina-Montenegro, M.A., Torres-Díaz, C., Perez, C., Gallardo, A., García-Velázquez, L., Hayes, P.E., Neuhauser, S., He, J.-Z. The global distribution and environmental drivers of the soil antibiotic resistome. (2022) *Microbiome*, 10 (1), art. no. 219. DOI: 10.1186/s40168-022-01405-w
- García-Velázquez, L., Gallardo, A., Ochoa, V., Gozalo, B., Lázaro, R., Maestre, F.T. Biocrusts increase the resistance to warming-induced increases in topsoil P pools. (2022) *Journal of Ecology*, 110 (9), pp. 2074-2087. DOI: 10.1111/1365-2745.13930
- Dacal, M., Delgado-Baquerizo, M., Barquero, J., Berhe, A.A., Gallardo, A., Maestre, F.T., García-Palacios, P. Temperature Increases Soil Respiration Across Ecosystem Types and Soil Development, But Soil Properties Determine the Magnitude of This Effect. (2022) *Ecosystems*, 25 (1), pp. 184-198.
- Blanco, G., Domínguez, L., Fernández, L., Martínez, F., González del Barrio, J.L., Frías, O., Cuevas, J.A. & Carrete, M. 2022. The decline of common birds exemplified by the Eurasian Jackdaw warns on strong environmental degradation. *Conservation*.
- Delgado-González, A., Cortés-Avizanda, A., Serrano, D., Arrondo, E., Duriez, O., Margalida, A., Carrete, M., Oliva-Vidal, P., Sourp, E., Morales-Reyes, Z., García-Barón, I., de la Riva, M., Sánchez-Zapata, J.A. & Donázar, J.A. 2022. Apex scavengers from different European populations converge at threatened savannah landscapes. *Scientific Reports*.
- Hernández-Brito, D., Carrete, M. and Tella, J.L. 2022. Annual Censuses and Citizen Science Data Show Rapid Population Increases and Range Expansion of Invasive Rose-Ringed and Monk Parakeets in Seville, Spain. *Animals*.
- Blanco, G., Morinha, F., Carrete, M. and Tella, J.L. 2022. Apparent Lack of Circovirus Transmission from Invasive Parakeets to Native Birds. *Int. J. Environ. Res. Public Health* 19, 3196.



- Blanco, G., Frías, O., Pitarch, A. and Carrete, M. 2022. Oral disease is linked to low nestling condition and brood size in a raptor species living in a highly modified environment. *Current Zoology*.
- Carrete, M., Hiraldo, F., Romero-Vidal, P., Blanco, G., Hernández-Brito, D., Sebastián-González, E., Díaz-Luque, J.A. and Tella, J.L. 2022. Worldwide distribution of antagonistic-mutualistic relationships between parrots and palms. *Frontiers in Ecology and Evolution*.
- Carrete, M., Clavero, M., Arrondo, E., Traveset, A., Bernardo-Madrid, R., Vilà, M., Blas, J., Nogales, M., Delibes, M., García-Rodríguez, A., Hernández-Brito, D., Romero-Vidal, P. and Tella, J.L. 2022. Emerging laws must not protect stray cats and their impacts. *Conservation Science and Practice*.
- Romero-Vidal, P., Carrete, M., Hiraldo, F., Blanco, G. and Tella, J.L. 2022. Confounding rules can hinder conservation: disparities in law regulation on domestic and international parrot trade within and among Neotropical countries. *Animals*.
- Cardador, L., Tella, J.L., Louvrier, J., Anadón, J.D., Abellán, P. & Carrete, M. 2022. Climate matching and anthropogenic factors contribute to the colonisation and extinction of local populations during avian invasions. *Diversity and Distribution*.
- Tella, J.L., Blanco, G. & Carrete, M. 2022. Recent Advances in Parrot Research and Conservation. *Diversity* 14, 419.
- Gómez-López, G., Martínez, F., Sanz-Aguilar, A., Carrete, M. & Blanco, G. 2022. Nestling sex ratio is unaffected by individual and population traits in the griffon vulture. *Current Zoology*, zoac046
- Pérez-García, J.M., Morant, J., Arrondo, E., Sebastián-González, E., Lambertucci, S.A., Santagneli, A., Margalida, A., Sánchez-Zapata, J.A., Blanco, G., Donázar, J.A., Carrete, M. & Serrano, D. 2022. Priority areas for conservation alone are not a good proxy for predicting the impact of renewable energy expansion. *Proc Natl Acad Sci USA*.
- Sáez-Ventura, Á.; López-Montoya, A.J.; Luna, Á.; Romero-Vidal, P.; Palma, A.; Tella, J.L.; Carrete, M.; Liébanas, G.M.; Pérez, J.M. 2022. Drivers of the Ectoparasite Community and Co-Infection Patterns in Rural and Urban Burrowing Owls. *Biology* 11, 1141.
- Romero-Vidal, P., Luna, A., Fernández-Gómez, L., Navarro, J., Palma, A., Tella, J.L. & Carrete, M. 2022. Intraspecific competition and individual behaviour but not urbanization affect the dietary patterns of a generalist avian predator. *Scientific Reports*.
- Morant, J., Arrondo, E., Sanchez-Zapata, J.A., Donázar, J.A., Cortés-Avizanda, A., de la Riva, M., Blanco, G., Martínez, F., Oltra, J., Carrete, M., Margalida, A., Oliva-Vidal, P., Martínez, J.M., Serrano, D. and Peréz-García, J.M. Large-scale movement patterns in a social vulture are influenced by seasonality, sex, and breeding region. *Ecology and Evolution*.
- Romero-Vidal, P., Toledo-Gonzalez, B., Bunn, L. , Blanco, G. , Hiraldo, F. , Bermúdez, A.O., Carrete, M. , Tella, J.L. 2023. Poaching sources and trade routes in Peru and Ecuador warn of the



unsustainable rural demand for preferred parrot species. *Conservation Science and Practice* e12936.

- Valeriano et al. 2023. Delineating vulnerability to drought using a process-based growth model in Pyrenean silver fir forests. *Forest Ecology and Management*. 541. 121069. <https://doi.org/10.1016/j.foreco.2023.121069>.
- Cobo-Simón et al. 2023. De novo transcriptome sequencing and gene co-expression reveal a genomic basis for drought sensitiveness and evidence of rapid local adaptation on Atlas cedar (*Cedrus atlantica*). *Frontiers in Plant Science*. 14. <https://doi.org/10.3389/fpls.2023.1116863>.
- Cobo-Simón et al. 2023. Contrasting transcriptomic patterns reveal a genomic basis for drought resilience in the relict fir *Abies pinsapo* Boiss. *Tree Physiology*. 43. 315–334. <https://doi.org/10.1093/treephys/tpac115>.
- Méndez-Cea et al. 2023. Tree-Level Growth Patterns and Genetic Associations Depict Drought Legacies in the Relict Forests of *Abies marocana*. *Plants*. 12, 873. <https://doi.org/10.3390/plants12040873>.
- Méndez-Cea et al. 2023. Weak genetic differentiation but strong climate-induced selective pressure toward the rear edge of mountain pine in north-eastern Spain. *Science of The Total Environment*. 858. 159778. <https://doi.org/10.1016/j.scitotenv.2022.159778>.
- Cortés-Molino et al. 2022. Unexpected resilience in relict *Abies pinsapo* Boiss forests to dieback and mortality induced by climate change. *Frontiers in Plant Science*. 13. <https://doi.org/10.3389/fpls.2022.991720>
- González de Andrés et al. 2022. The role of nutritional impairment in carbon-water balance of silver fir drought-induced dieback. *Global Change Biology*. 28, 4439– 4458. <https://doi.org/10.1111/gcb.16170>.
- García-García et al. 2022. Challenges and Perspectives in the Epigenetics of Climate Change-Induced Forests Decline. *Frontiers in Plant Science*. 12. <https://doi.org/10.3389/fpls.2021.797958>.
- Candel-Pérez et al. 2022. Forest structure drives the expected growth of *Pinus nigra* along its latitudinal gradient under warming climate. *Forest Ecology and Management*. 505. 119818. <https://doi.org/10.1016/j.foreco.2021.119818>.
- Ben-Said et al. 2022. Spatial patterns and species coexistence in mixed *Abies marocana*-*Cedrus atlantica* forest in Talassemtane National Park. *Forest Ecology and Management*. 506. 119967. <https://doi.org/10.1016/j.foreco.2021.119967>.
- Gazol et al. 2022. Tree Growth Response to Drought Partially Explains Regional-Scale Growth and Mortality Patterns in Iberian Forests. *Ecological Applications*. 32(5): e2589. <https://doi.org/10.1002/eap.2589>.



- Cerman, K., Rajković, D., Topić, B., Topić, G., Shurulinkov, P., Mihelič, T., Delgado, J.D. 2022. Environmental Niche Modelling Predicts a Contraction in the Potential Distribution of Two Boreal Owl Species under Different Climate Scenarios. *Animals* 12 (22), 3226. <https://doi.org/10.3390/ani12223226>
- Morelli, F., Benedetti, Y., Szkudlarek, M., Abou Zeid, F., Delgado, J.D., Kaczmarski, M. 2023. Potential hotspots of amphibian roadkill risk in Spain. *Journal of Environmental Management* 342: 118346. <https://doi.org/10.1016/j.jenvman.2023.118346>

Área de Física Aplicada

- B. Almeida-Zamora, J.J. Cobos-Martínez, A. Bashir, K. Raya, J. Rodríguez-Quintero and J. Segovia, “Light-front Wave Functions of Vector Mesons in an Algebraic Model”, *Phys. Rev. D*107 (2023) 074037.
- P.G. Ortega, J. Segovia, D.R. Entem and F. Fernández, “Nature of the doubly-charmed tetraquark \mathbf{T}_{cc}^{++} in a constituent quark model”, *Phys. Lett. B*841 (2023) 137918.
- A. Duenas-Vidal and J. Segovia, “Arising of trapped surfaces with non-trivial topology from colliding shock waves”, *Phys. Rev. D*107 (2023) 024008.
- U. Taboada-Nieto, P.G. Ortega, D.R. Entem F. Fernández and J. Segovia, “Kaon spectrum revisited”, *Eur. Phys. J. A*59 (2023) 40.
- M.C. Gordillo, F. de Soto and J. Segovia, “ $X(3872)$'s excitation and its connection with production at hadron colliders”, *Phys. Rev. D*106 (2022) 094004.
- G. Yang, J. Ping and J. Segovia, “Fully-charm and -bottom pentaquarks in a Lattice-QCD inspired quark model”, *Phys. Rev. D*106 (2022) 014005.
- B. Martín-González, P. G. Ortega, D. R. Entem, F. Fernández and J. Segovia , “Towards the discovery of novel B_c states: radiative and hadronic transitions”, *Phys. Rev. D*106 (2022) 054009.
- G. Yang, J. Ping and J. Segovia, “Bottomonium-like tetraquarks in a chiral quark model”, *Phys. Rev. D*106 (2022) 014021.
- L. Liu, C. Chen, Y. Lu, C.D. Roberts and J. Segovia, “Composition of low-lying $J=\frac{3}{2}^{\pm}$ Δ -baryons”, *Phys. Rev. D*105 (2022) 114047.



- J.M. Alcaraz-Pelegrina and M.C. Gordillo. "Diffusion Monte Carlo calculations of fully-heavy compact hexaquarks" Phys. Rev. D **106** 114028 1-6 (2022).
- M.C. Gordillo and J.Boronat "H₂ superglass on an amorphous carbon substrate" Phys. Rev. B **107** L060505_1-5 (2023).
- M.C. Gordillo, R. Rodríguez-García and J.Boronat "Phases of ⁴He and H₂ adsorbed on a single carbon nanotube" Phys. Rev. B. **107**, 174518 (2023).
- F. Pinto-Gómez, F. De Soto, M.N. Ferreira, J. Papavassiliou, J. Rodríguez-Quintero "Lattice three-gluon vertex in extended kinematics: Planar degeneracy" Phys.Lett.B 838 (2023) 137737
- A.C. Aguilar, F. De Soto, M.N. Ferreira, J. Papavassiliou, F. Pinto-Gómez, C.D. Roberts, J. Rodríguez-Quintero "Schwinger mechanism for gluons from lattice QCD" Phys.Lett.B 841 (2023) 137906

Área de Física de la Tierra

- Bacelar Valente, M. (2022). The Faithfulness Problem. In Principia: an international journal of epistemology (Vol. 26, Issue 3). Universidade Federal de Santa Catarina (UFSC). <https://doi.org/10.5007/1808-1711.2022.e84395>
- Bacelar Valente, M. (2022). Do All Languages Share the Same Conceptual Structure? In Cognitive Semantics (Vol. 8, Issue 2, pp. 159–180). Brill. <https://doi.org/10.1163/23526416-08020001>
- Hempelmann, N., Ehbrecht, C., Plesiat, E., Hobona, G., Simoes, J., Huard, D., Smith, T. J., McKnight, U. S., Pechlivanidis, I. G., & Alvarez-Castro, C. (2022). DEPLOYMENT OF AI-ENHANCED SERVICES IN CLIMATE RESILIENCE INFORMATION SYSTEMS. In The International Archives of the Photogrammetry, Remote Sensing and Spatial Information Sciences: Vol. XLVIII-4/W1-2022 (pp. 187–194). Copernicus GmbH. <https://doi.org/10.5194/isprs-archives-xlviii-4-w1-2022-187-2022>

Área de Geodinámica Externa

- Halmos, L., Delgado, J., Rodríguez-Rodríguez, M., Jiménez-Bonilla, A., Díaz-Azpiroz, M. (2022). Physicochemical characteristics of playa-lake sediments located in the western External Betics. Geogaceta 72, 39-42.



- Moral, F., Expósito, I., Jiménez-Bonilla, A. (2022). Trazado y depósitos aluviales del Guadalquivir medio e implicaciones tectónicas (Córdoba y Jaén). *Geogaceta* 72, 43-46.
- Balanyá, J.C., Expósito, I., Jiménez-Bonilla, A., Díaz-Azpiroz, M., Sánchez, M., Crespo-Blanc (2022). Desacoplamiento de la deformación en la base de la lámina cabalgante del Dominio de Alborán (Béticas Occidentales). *Geogaceta* 72, 23-26.
- Jiménez-Bonilla, A., Expósito, I., Díaz-Azpiroz, M., Balanyá, J.C., Crespo-Blanc, A. (2022). Strain partitioning and localization due to detachment heterogeneities in fold-and-thrust belts of progressive arcs: Results from analogue modelling. *Tectonics* 41(12).
- Jiménez-Bonilla, A.; Díaz-Azpiroz, M. y Rodriguez-Rodriguez, M. Tectonics may also affect closed watersheds used to monitor climate change and human activity effects. 2022. *Terra Nova*. 35 (1).
- Treviño, J., Rodríguez-Rodríguez, M., Montes-Vega, M. J., Aguilera, H., Fernández-Ayuso, A., y Fernández-Naranjo, N. 2023. Wavelet Analysis on Groundwater, Surface-Water Levels and Water Temperature in Doñana National Park (Coastal Aquifer in Southwestern Spain). *Water*. 15 (4), 796. <https://doi.org/10.3390/w15040796>
- A. Fernández-Ayuso, C. Kohfahl, H. Aguilera, Rodriguez-Rodriguez, M., F. Ruiz-Bermudo, C. Serrano-Hidalgo, y C. Romero-Álvarez. 2023. Control of trace metal distribution and variability in an interdunal wetland, *Science of the Total Environment*. 857 (3), <https://doi.org/10.1016/j.scitotenv.2022.159409>
- Yanes, J.L. y Moral, F. 2022. Relief and climate influence on isotopic composition of Atlantic-Mediterranean karst spring waters (Andalusia, southern Spain). *Hydrological Processes*, 36(9), e14669. <https://doi.org/10.1002/hyp.14669>.
- Expósito, I., Jiménez-Bonilla, A., Delchiaro, M., Yanes, L.L., Balanyá, J.C., Moral, F., and Della Setta, M. 2022. Geomorphic signature of segmented relief rejuvenation in the Sierra Morena, Betic forebulge, Spain. *Earth Surf. Dynam.*, 10, 1017–1039. <https://doi.org/10.5194/esurf-10-1017-2022>.

Área de Geodinámica Interna

- Balanyá, J.C., Expósito, I., Jiménez-Bonilla, A., Díaz-Azpiroz, M., Sánchez-Gómez, M., Crespo-Blanc, A. (2022). Desacoplamiento de la deformación en la base de la lámina cabalgante del Dominio de Alborán (Béticas Occidentales). *Geogaceta*, 72, 23-26.
- Expósito, I., Jiménez-Bonilla, A., Delchiaro, M., Yanes, J. L., Balanyá, J. C., Moral-Martos, F., Della Setta, M.: Geomorphic signature of segmented relief rejuvenation in the Sierra Morena,



Betic forebulge, Spain, *Earth Surf. Dynam.*, 10, 1017–1039. <https://doi.org/10.5194/esurf-10-1017-2022>, 2022

- Halmos L., Delgado J., Rodríguez-Rodríguez M., Jiménez-Bonilla A., Díaz-Azpiroz M. (2022). Physicochemical characteristics of playa-lake sediments located in the western External Betics, *Geogaceta* 72, 43-46.
- Jiménez-Bonilla, A., Díaz-Azpiroz, M., & Rodríguez-Rodríguez M.. (2023). Tectonics may affect closed watersheds used to monitor climate change and human activity effects. *Terra Nova*, 35, 58– 65. <https://doi.org/10.1111/ter.12629>.
- Jiménez-Bonilla, A., Expósito, I. E., Díaz-Azpiroz, M., Balanyá, J. C., & Crespo-Blanc, A. (2022). Strain partitioning and localization due to detachment heterogeneities in fold-and-thrust belts of progressive arcs: Results from analog modeling. *Tectonics*, 41, e2021TC006955. <https://doi.org/10.1029/2021TC006955>
- Moral F., Expósito I.& Jiménez-Bonilla A. (2022). Trazado y depósitos aluviales del Guadalquivir medio e implicaciones tectónicas (Córdoba y Jaén), *Geogaceta* 72, 43-46.

Área de Química Física

- Matías Valdés, Alejandro Hernandez Martínez, Yudania Sánchez, Robert Fonoll, Marcel Placidi, Victor Izquierdo-Roca, Antonio Cabas Vidani, Matteo Valentini, Alberto Mittiga, Paul Pistor, Claudia Malerba, Edgardo Saucedo. "A new approach for alkali incorporation in Cu₂ZnSnS₄ solar cells", *Journal of Physics: Energy*. 4, pp. 044008 (2022). DOI: 10.1088/2515-7655/ac96a4
- Guc, Bailo, Fonoll-Rubio, Atlan, Placidi, Jackson, Hariskos, Alcobe, Pistor, Becerril-Romero, Perez-Rodriguez, Ramos, Izquierdo-Roca. Evaluation of defect formation in chalcopyrite compounds under Cu-poor conditions by advanced structural and vibrational analyses. *Acta Materialia*. 223, pp. 117507 (2022). DOI: 10.1016/j.actamat.2021.117507
- Robert Heidrich, Karl L. Heinze, Sebastian Berwig, Jie Ge, Roland Scheer, Paul Pistor. "Impact of dynamic co-evaporation schemes on the growth of methylammonium lead iodide absorbers for inverted solar cells". *Scientific Reports*, 12 - 1, pp. 19167 (2022). DOI: 10.1038/s41598-022-23132-w
- Alejandro Hernández-Martínez, Sergio Giraldo, Xavier Alcobé, Ignacio Becerril-Romero, Marcel Placidi, Victor Izquierdo-Roca, Paul Pistor, Alejandro Pérez-Rodríguez, Edgardo Saucedo, Matías Valdés, Matías Valdés. "Kinetics and phase analysis of kesterite compounds: Influence of chalcogen availability in the reaction pathway". *Materialia*. 24, pp. 101509 (2022). DOI: 10.1016/j.mtla.2022.101509



- Thomas Burwig, Karl Heinze, Paul Pistor. "Thermal decomposition kinetics of FAPbI₃ thin films". *Physical Review Materials*. 6, pp. 065404 (2022). DOI: 10.1103/PhysRevMaterials.6.065404
- [Aviles-Moreno, JR](#); Gamez F.; [Berden, G](#); [Oomens, J](#); [Martinez-Haya, B](#), Inclusion complexes of the macrocycle nonactin with benchmark protonated amines: aniline and serine. *Physical Chemistry Chemical Physics* (2022) 24, 8422-8431
- [Aviles-Moreno, JR](#); [Berden, G](#); [Oomens, J](#); [Martinez-Haya, B](#), Insights into the binding of arginine to adenosine phosphate from mimetic complexes. *Physical Chemistry Chemical* (2022) 24, 27136-27145
- [Martinez-Haya, B](#); [Aviles-Moreno, JR](#); [Gamez, F](#); [Martens, J](#); [Oomens, J](#); [Berden, G](#), A Dynamic Proton Bond: MH⁺-H₂O \longleftrightarrow M-H₃O⁺ Interconversion in Loosely Coordinated Environments, *Journal of Physical Chemistry Letters* (2023), 14, 1294-1300
- Dena Pourjafari, Nidia G. García-Peña, Wendy Y. Padron-Hernández, Diecenia Peralta-Domínguez, Alejandra María Castro-Chong, Mahmoud Nabil, Roberto C. Avilés-Betanzos and Gerko Oskam. "Functional Materials for Fabrication of Carbon-Based Perovskite Solar Cells: Ink Formulation and Its Effect on Solar Cell Performance" (Review Article). *Materials* 16, 3917 (39 pp) (2023). <https://doi.org/10.3390/ma16113917>
- Francisco J. Peón-Díaz, Rodrigo Segura del Río, Samuel Hevia, Fernanda Olivares, Juan Carlos Expósito-Gálvez, Renán Escalante, Karen Valadez-Villalobos, Antonio J. Riquelme, Gerko Oskam, and Ricardo Henríquez. "The effect of oxidative functionalization of carbon nanotubes on the morphological, optical, and photoelectrochemical properties of modified titanium dioxide photoanodes". *J. Mater. Sci.* 58, 5372-5388 (2023). <https://doi.org/10.1007/s10853-023-08351-4>
- Roberto Villarroel, Dario Zambrano-Mera, Rodrigo Espinoza-González, Katherine Paredes- Gil, Stefano Pantaleone, Luis Ballesteros, Gerko Oskam, José A. García-Merino, Samuel A. Hevia, Guillermo González-Moraga. "Structural and photoelectrochemical dynamics of in-situ hydrogenated anatase TiO₂ thin films grown by DC reactive magnetron sputtering". *Appl. Surf. Sci.* 607, 155023 (2023). <https://doi.org/10.1016/j.apsusc.2022.155023>
- Carlos A. Gonzalez-Flores, Dena Pourjafari, Renan Escalante, Esdras J. Canto-Aguilar, Alberto Vega Poot, José María Andres Castán, Yann Kervella, Renaud Demadrille, Antonio J. Riquelme, Juan A. Anta, and Gerko Oskam. "Influence of Redox Couple on the Performance of ZnO Dye Solar Cells and Minimodules with Benzothiadiazole-Based Photosensitizers". *ACS Appl. Energy Mater.* 5, 14092 - 14106 (2022). <https://doi.org/10.1021/acsaelm.2c02609>



- Rodrigo García-Rodríguez, Antonio J. Riquelme, Matthew Cowley, Karen Valadez-Villalobos, Gerko Oskam, Laurence J. Bennett, Matthew J. Wolf, Lidia Contreras-Bernal, Petra J. Cameron, Alison B. Walker, and Juan A. Anta. "Inverted Hysteresis in n-i-p and p-i-n Perovskite Solar Cells". *Energ. Technol.* 2200507 (9 pp) (2022). <https://doi.org/10.1002/ente.202200507>
- Stijn Lammar, Renán Escalante, Antonio J. Riquelme, Sandra Jenatsch, Beat Ruhstaller, Gerko Oskam, Tom Aernouts and Juan A. Anta. "Impact of non-stoichiometry on ion migration and photovoltaic performance of formamidinium- based perovskite solar cells". *J. Mater. Chem. A* 10, 18782–18791 (2022). <https://doi.org/10.1039/d2ta04840j>
- Antonio J. Riquelme, Karen Valadez-Villalobos, Pablo P. Boix, Gerko Oskam, Iván Mora-Seró and Juan A. Anta. "Understanding equivalent circuits in perovskite solar cells. Insights from drift-diffusion simulation". *Phys. Chem. Chem. Phys.* 24, 15657–15671 (2022). <https://doi.org/10.1039/d2cp01338j>
- Dominika O. Wasik, Ana Martín-Calvo, Juan J. Gutiérrez-Sevillano, David Dubbeldam, Thijs J. H. Vlugt, y Sofía Calero. Enhancement of Formic Acid Production from Carbon Dioxide Hydrogenation Using Metal-Organic Frameworks: A Molecular Simulation Study. *Chemical Engineering Journal*, 2023, volume 467, 143432. <https://doi.org/10.1016/j.cej.2023.143432>
- Xiucheng Huang, Ana Martín-Calvo, Martijn J.J. Mulder, Sjoerd C.J. van Acht, Juan J. Gutierrez-Sevillano, Julio C. Garcia-Navarro, y Sofía Calero. Effect of Zeolitic Imidazolate Framework Topology on the Purification of Hydrogen from Coke Oven Gas. *ACS Sustainable Chemistry & Engineering*, 2023, 11, 21, 8020–8034. <https://doi.org/10.1021/acssuschemeng.2c07006>
- Delgado Campos, Andres, Cuetos Alejandro, Influence of homeostatic mechanisms of bacterial growth and division on structural properties of microcolonies: A computer simulation study. *Phys. Rev. E* 103, 034402, (2022)
- Rodriguez-Rivas, Alvaro, Patti, Alessandro, Cuetos, Alejandro. Dynamics in field-induced biaxial nematic liquid crystals of board-like particles. *J. Mol. Liq.* 367, 120371 (2022)
- Xiucheng Huang, Ana Martín-Calvo, Martijn JJ Mulder, Sjoerd CJ van Acht, Juan José Gutiérrez-Sevillano, Julio C García-Navarro, Sofía Calero "Effect of Zeolitic Imidazolate Framework Topology on the Purification of Hydrogen from Coke Oven Gas" *ACS Sustainable Chem. Eng.* 2023, 11, 21, 8020–8034



- Acuna-Yeomans, E; Gutierrez-Sevillano, JJ; Calero, S and Dubbeldam, D. "Evaluation of ZIF-8 flexible force fields for structural and mechanical properties" *Microporous and mesoporous*, 348, 112406, (2023), DOI: 10.1016/j.micromeso.2022.112406.
- Zhakisheva,B.; Gutiérrez-Sevillano,JJ. and Calero S. "Ammonia and water in zeolites: Effect of aluminum distribution on the heat of adsorption" *Separation and Purification Technology*, Volume 306, Part A, 1 February 2023, 122564
- Jajko, G; Calero, S.; Kozyra, P.; Makowski, W.; Sławek, A.; Gil, B.; and Gutiérrez-Sevillano, JJ; Defect-induced tuning of polarity-dependent adsorption in hydrophobic–hydrophilic UiO-66, *Communications Chemistry*, 5 (1), 1-9, 2022
- F.G. Moscoso, L.M. Rodriguez-Albelo, A.R. Ruiz-Salvador, Tânia Lopes-Costa, J.M. Pedrosa, Enhancement of the intrinsic fluorescence of ZIF-8 via post-synthetic cation exchange with Cd²⁺ and its incorporation into PDMS films for selective sulfide optical sensing, *Materials Today Chemistry*, 2023, 28, 101366 <https://doi.org/10.1016/j.mtchem.2022.101366>
- S. R. G. Balestra, B. Martínez-Haya, N. C. Hernández, D. W. Lewis, S. M. Woodley, R. Semino, G. Maurin, A. R. Ruiz-Salvador and S. Hamad, Nucleation of Zeolitic Imidazolate Frameworks: from molecules to nanoparticles, *Nanoscale*, 2023, 15, 3504-3519 DOI: <https://doi.org/10.1039/D2NR06521E>
- D. De la Lama-Calvente, M. J. Fernández-Rodríguez, M. Ballesteros, A. R. Ruiz-Salvador, F. Raposo, J. C. García-Gómez and R. Borja, Turning an invasive alien species into a valuable biomass: Anaerobic digestion of *Rugulopteryx okamurae* after thermal and new developed low-cost mechanical pretreatments, *Sci. Total Environ.*, 2023, 856, 158914, <https://doi.org/10.1016/j.scitotenv.2022.158914>
- J. M. Ortiz-Roldan, S. R. G. Balestra, R. Bueno-Perez, S. Calero, E. Garcia-Perez, C. R. A. Catlow, A. R. Ruiz-Salvador, S. Hamad, Understanding the stability and structural properties of Ordered Nanoporous Metals towards their rational synthesis, *Proc. R. Soc. A*, 2022, 478, 20220201, <https://doi.org/10.1098/rspa.2022.0201>
- M. Urbiztondo, A. Ramirez, J.L. Hueso, J. Santamaria, A.R. Ruiz-Salvador and S. Hamad, *Nanoscale*, 2022, 14, 7332-7340, Unravelling the key factors in the chlorine-promoted epoxidation of ethylene over a silver–copper oxide nanocatalyst, <https://doi.org/10.1039/D2NR00702A>
- J. M. Ortiz-Roldan, F. Montero-Chacón, E. Garcia-Perez, S. Calero, A. R. Ruiz-Salvador and S. Hamad, Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via



Molecular Dynamics Simulations, , Advanced Composite Materials, 31 (2022) 485-504,
<https://doi.org/10.1080/09243046.2021.2001988>

- Pablo Sánchez-Palencia, Said Hamad, Pablo Palacios, Ricardo Grau-Crespo ORCID logo e and Keith T. Butler. Spinel nitride solid solutions: charting properties in the configurational space with explainable machine learning, Digital Discovery, 2022,1, 665-678
- Fátima Guerrero, Victoria Pulido, Said Hamad, Pedro Aljama, Alejandro Martín-Malo and Carolina Carrillo-Carrión, Incorporating zeolitic-imidazolate framework-8 nanoparticles into kidney scaffolds: a first step towards innovative renal therapies ,Nanoscale, 2022,14, 17543-17549