Fecha del CVA	21/01/2024

Parte A. DATOS PERSONALES

Nombre	Alberto		
Apellidos	Fraile García		
Sexo	No Contesta	Fecha de Nacimiento	
DNI/NIE/Pasaporte			
URL Web	https://www.researchgate.net/profile/Alberto-Fraile-5		
Dirección Email			
Open Researcher and Contributor ID (ORCID)	0000-0003-2646-5159		

A.1. Situación profesional actual

Puesto	Post-Doctoral Research Officer		
Fecha inicio	2023		
Organismo / Institución	Materials Physics Center		
Departamento / Centro			
País		Teléfono	
Palabras clave	Dinámica molecular; Simulacion numerica; Diseño asistido por ordenador; Caracteristicas de los materiales		

A.2. Situación profesional anterior (incluye interrupciones en la carrera investigadora - indicar meses totales, según texto convocatoria-)

Periodo	Puesto / Institución / País
2021 - 2023	Advanced Reactor Materials Research Officer / Nuclear Futures Institute. Bangor University (UK)
2017 - 2020	Postdoctoral Researcher Fellow / Advanced Materials Group, Czech Technical University / República Checa
2013 - 2016	Postdoctoral Researcher fellow / Crete Center of Quantum Complexity & Nanotechnology (CCQCN), University of Crete, Iraklion / Grecia
2013 - 2013	Visiting researcher / Queen's University Belfast (UK) / Reino Unido
2009 - 2013	PhD Student / Instituto de Fusion Nuclear, Madrid / España
2003 - 2009	Assistant at the Laboratory of Magnetism / Universidad de Zaragoza / España

A.3. Formación académica

Grado/Master/Tesis	Universidad / País	Año
PhD in Nuclear Engineering (Cum Laude). Atomistic simulation of liquid metals and alloys for nuclear fusion reactors. Universidad Politécnica de Madrid, Instituto de Fusión Nuclear (Madrid, SP	Instituto de Fusión Nuclear / España	2013
Master's degree on Solid State Physics	Universidad de Zaragoza / España	2005
Licenciado en Física Especialidad Física Fundamental	Universidad de Zaragoza / España	2001

Parte B. RESUMEN DEL CV

2013. PhD in Nuclear Engineering (Cum Laude). Atomistic simulation of liquid metals and alloys for nuclear fusion reactors. Instituto de Fusión Nuclear (Madrid, SP).
2005. Master's degree on Solid State Physics. University of Zaragoza (Zaragoza, SP).
2002. Bachelor's degree on Physics. University of Zaragoza (Zaragoza, SP)

In 2013 I finished my PhD in the Institute of Nuclear Fusion, Madrid. The main goal was to use molecular dynamics (MD) to study different problems related with breeding blankets. Our research was carried out in collaboration with Los Alamos National Laboratory, where I worked for 7 months. After my PhD I was invited by Prof J. Kohanoff to join the Atomistic Simulation Center at Queen's University Belfast, where I studied the effect of shock waves in biological media using ab initio MD.
In the next 3 years, I worked in the University of Heraklion where we analyzed the non-linear physics of 2D materials using atomistic simulations.
In Czech Technical University Prague my research focused on the atomistic design and simulation of nanostructured materials.
Recently, we examined the damage produced by hypervelocity impacts in tungsten. The first paper appeared in Nuclear Fusion, (cover of the journal, highlighting the importance of the work), and two more papers are in progress. Then I worked in the Nuclear Futures Institute (Bangor, UK) where I was involved in several projects (experimental and modelling), from high entropy alloys to plasma facing materials. In 2021 I was awarded with £50,000 (Bangor University Innovation and Impact Award) for my project "Design of Novel HEA Coatings for Extreme Environments". In 2023 I was granted with the Royce Undergraduate Internship Scheme (£5,000) for a similar project.
I worked as consultant for Westinghouse, Jacobs, Tribosonics and Turkish Aerospace.
I wrote 14 proposals for computational resources in HPC facilities. (>26 000 000 CPU/hs in IT4I, Supercomputing facility (Ostrava, CZR), as PI or Co-PI.
In Crete, I co-supervised two master students. Now I am finishing the co-supervision of a PhD student in Prague.
Before my PhD, I worked five years in the Laboratory of Magnetism at the University of Zaragoza and in the ISIS neutron spallation source (UK).

In November 2023 I joined the Materials Phisics Center (UPV, San Sebastian). The "Electronic Excitations in Surfaces & Nanostructures" group is mostly devoted to the theoretical study of electron dynamics in solids, surfaces and materials of technological interest. Electron dynamics in different systems is investigated, with particular emphasis on ultrafast processes. My research is carried out mainly using Density Functional Theory (DFT) simulations and Machine Learning (ML) techniques.
My list of skills can be summarized as follows. Simulation: Atomistic simulation (liquid metals, metallic systems, alloys, shock waves, graphene) with classical and first-principles MD. LAMMPS, VASP, CP2K. Ovito, VESTA, fortran, python, Mathematica, Linux. Experimental: Transport & magnetic measurements, SQUID, PPMS, magnetostriction (capacitive cells, strain gauge), neutron techniques, X-ray diffraction, SEM, AFM.

Parte C. LISTADO DE APORTACIONES MÁS RELEVANTES

C.1. Publicaciones más importantes en libros y revistas con "peer review" y conferencias

AC: Autor de correspondencia; (nº x / nº y): posición firma solicitante / total autores. Si aplica, indique el número de citaciones

1 **Artículo científico**. 2023. Assessing Li accommodation at amorphous ZrO2 grain boundaries. Journal of Nuclear Materials. Elsevier.
2 **Artículo científico**. Ramin; Alexander; Alberto. 2023. A stochastic reaction–diffusion modeling investigation of FLASH ultra-high dose rate response in different tissues. Frontiers in Physics. Medical Physics.11-331.
3 **Artículo científico**. 2023. High-entropy Fe-Cr-Ni-Co-(Cu) coatings produced by vacuum electro-spark deposition for marine and coastal applications. Surface and Coatings Technology. 453-129136.
4 **Artículo científico**. Alberto; Prashant. 2022. Analysis of hypervelocity impacts: the tungsten case. Nuclear Fusion. 62-2.

5 **Artículo científico**. Pablo; Julien; Svetoslav; Alberto. 2022. Atomistic simulations of magnetoelastic effects on sound velocity. Physical Review B. 105-13.
6 **Artículo científico**. Alex; Jack; Alberto. 2022. Defect behaviour in the MoNbTaVW high entropy alloy (HEA). Results in Materials. 15.
7 **Artículo científico**. Jack; Lee; Alberto. 2022. Predicting the thermal expansion of BCC high entropy alloys in the Mo-Nb-Ta-Ti-W system. Journal of Physics: Energy. 4-3.
8 **Artículo científico**. VK; Alberto. 2021. Crystal electric field and possible coupling with phonons in Kondo lattice CeCuGa3. Physical Review B. 104-17.
9 **Artículo científico**. Alberto; Osame; Prashant. 2021. Prime numbers and random walks in a square grid. Physical Review E. 104-5.
10 **Artículo científico**. Hakan; Alberto. 2020. Deformation-Controlled Design of Metallic Nanocomposites. ACS Applied Materials & Interfaces. 11-49.
11 **Artículo científico**. Alberto; Roberto; Daniel. 2020. Jacob's Ladder: Prime Numbers in 2D. Mathematical and Computational Applications. 25-1.
12 **Artículo científico**. Andrey; Alberto. 2020. Mechanisms of friction and wear reduction by h-BN nanosheet and spherical W nanoparticle additives to base oil: Experimental study and molecular dynamics simulation. Tribology International. 151.
13 **Artículo científico**. Alberto; Tomas. 2020. Volume and pressure of helium bubbles inside liquid Pb16Li. A molecular dynamics study. Nuclear Fusion. 60-4.
14 **Artículo científico**. Alberto; Maeve; Jorge. 2019. First principles simulation of damage to solvated nucleotides due to shock waves. The Journal of Chemical Physics. 150-1.
15 **Artículo científico**. Alberto; Emmanouil. 2018. Cellular Automata and Artificial Brain Dynamics. Mathematical and Computational Applications. 23-4.
16 **Artículo científico**. Alberto; Emmanuel N. 2016. Long-lived discrete breathers in free standing graphene. Chaos, Solitons & Fractals. 87.
17 **Artículo científico**. Franz; Alberto. 2015. Experimental evidence for a dynamical crossover in liquid aluminium. Journal of Physics: Condensed Matter. 27-45.
18 **Artículo científico**. D T; Cesar; Alberto. 2015. Muon spin rotation and neutron scattering study of the non-centrosymmetric tetragonal compound CeAuAl3. Physical Review B. 91-13.
19 **Artículo científico**. VK; DT. 2015. Neutron scattering and SR studies on a Kondo lattice heavy fermion CeRuSn 3. Journal of Physics: Conference Series. 592-1.
20 **Artículo científico**. Alberto; Santiago. 2014. Interatomic potential for the compound-forming Li–Pb liquid alloy. Journal of Nuclear Materials. 448-1-3.
21 **Artículo científico**. Alberto; Santiago. 2013. Atomistic molecular point of view for liquid lead and lithium in Nuclear Fusion technology. Journal of Nuclear Materials. 440-1-3.
22 **Artículo científico**. Alberto; Santiago; José Manuel. 2012. Molecular Dynamics Simulations of Lead and Lithium in Liquid Phase. Fusion Science and Technology. Taylor & Francis. pp.77-82.
23 **Artículo científico**. DT; A. 2012. Vibron quasi-bound state in the non-centrosymmetric tetragonal heavy fermion compound CeCuAl3. Physical Review Letters. 108-21.
24 **Artículo científico**. VK; DT. 2011. Complex magnetic behaviour in the novel Kondo lattice compound CeRhSn3. Journal of Physics: Condensed Matter. 23-27.
25 **Artículo científico**. Cesar; Agustin. 2010. Study of 4f hybridization in CeNiX with X = Sn δ Ge 1−δ , 0≤δ≤1. Journal of magnetism and magnetic materials. 322-9-12.
26 **Artículo científico**. DT; AM. 2008. Crystal field excitations in the cubic compound Ce3Rh4Sn13. Physica B: Condensed Matter. 403-5-9.
27 **Artículo científico**. Alberto; Agustin. 2007. Kondo, fluctuation valence and non-Fermi liquid behaviors in CeNiSn1−xGex (0□x□1). Journal of Magnetism and Magnetic Materials. 310-2.
28 **Artículo científico**. Luis; Miguel; Alberto. 2007. Magnetoelastic Nature of the Dodecagonal Anisotropy in Holmium Metal. Physical Review Letters. 98-26.

C.2. Congresos

1 Analysis of hypervelocity impacts: the tungsten case.. LAMMPS Workshop and Symposium. August 8-11, (2023). Sandia National Lab. 2023.

2 Hypervelocity dust impacts on plasma facing materials. Symposium on Fusion Engineering (SOFE) Oxford 9th - 13th July (2023). UKAEA. 2023. Reino Unido.
3 Hypervelocity dust impacts on plasma facing materials through molecular dynamics simulations. 19th International Conference on Plasma-Facing Materials and Components (PFMC-19) Bonn, Germany. 22 – 26 May 2023. 2023. Alemania.
4 Al2O3 coatings for Lead Fast Reactors.. SAM Corrosion Model Workshop. 9-10 March 2023.. Argone NL, Westinhouse, Virginia Tech and Bangor University. 2023.
5 Liquid lead embrittlement through molecular dynamics simulations. NuMat 2022: The Nuclear Materials Conference. 2022. Bélgica.
6 Hypervelocity Impacts on Plasma Facing Materials through MD Simulations. 32nd Symposium on Fusion Technology 18–23 September 2022. 2022. Croacia.
7 Molecular dynamics simulation of hypervelocity impacts; Tungsten on tungsten. 15th COSIRES. 2022. Francia.
8 Volume and pressure of helium bubbles inside liquid Pb16Li. A molecular dynamic study. 1st Spanish Fusion HPC Workshop 2020. 2020.
9 Control of microstructural evolution of bimetallic Janus particles. Liquid and Amorphous Metals conference (LAM), 17th edition. 2019. Francia.
10 Interfaces and mechanisms: a MD approach to fine tuning manipulation of mechanical properties. ICMCTF 2019. 2019. Estados Unidos de América.
11 MD approach to fine tuning manipulation of interfaces. YUCOMAT 2018. 2018. Montenegro.
12 CVD layer growth of Nb-Zr layers; Molecular Dynamics analysis. E-MRS Spring Meeting. 2017. Francia.
13 Non-destructive tuning of thermal conductivity of graphene: A molecular dynamics study. Flatlands beyond graphene. 2016. Eslovenia.
14 Effect of Discrete Breathers in the Thermal Conductivity of Graphene. CECAM Workshop. Hot nanostructures: thermal transport and radiation at the nanoscale. 2015. Alemania.
15 Long-lived discrete breathers in graphene. Nanotechnology 2015. 2015. Grecia.
16 Molecular dynamics simulation of discrete breathers in graphene. International RMS 2014. 2014. Francia.
17 Exploring the limits of Classical Molecular Dynamics: Li and Pb liquid metals under pressure. New insights on metals under extreme conditions. 2012. Francia.
18 Molecular dynamics simulation of hydrogen diffusion in liquid metals. Trends on Nanotechnology, TNT 2012. 2012. España.
19 Liquid metals and Lithium Lead Eutectic alloys: Molecular dynamics simulations. ICOPS/SOFE. 2011. Estados Unidos de América.
20 Lithium lead eutectic alloys: A Multiscale approach from QMD to CMD. Joint ICTP/IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials. 2010. Italia.

C.3. Proyectos o líneas de investigación

1 **Proyecto**. Design of High Entropy Alloys for extreme environments. Royce Undergraduate Research Internship Scheme 2023. (Bangor University, Nuclear Futures Institute). 01/06/2023-31/07/2023. 4.000 €.
2 **Proyecto**. Design and Synthesis of Novel High Entropy Alloy Coatings for Extreme Environments. Bangor University Innovation and Impact Award. Fraile Garcia PI. (Nuclear Futures Institute, Bangor University). 01/04/2022-01/04/2023. 55.000 €. Investigador principal. PI of the project. Supervision, Funding, Co-writing manuscript and analysis.