

## Part A. PERSONAL INFORMATION

		CV date	15/10/2024
First and Family name	Felipe Jiménez Blas		
Social Security, Passport, ID number		Age	
Researcher codes	Open Researcher and Contributor ID (ORCID**)	0000-0001-9030-040X	
	SCOPUS Author ID (*)	56910383400	
	WoS Researcher ID (*)	L-3762-2014	

### A.1. Current position

Name of University/Institution	Universidad de Huelva		
Department	Centro de Investigación en Química Sostenible - CIQSO		
Address and Country	Edificio Robert H Grubbs, Campus de El Carmen, Universidad de Huelva, 21007 Huelva, Spain		
Phone number	959219796	E-mail	<a href="mailto:felipe@uhu.es">felipe@uhu.es</a>
Current position	Catedrático de Universidad (Física Aplicada)	From	19/10/2017
Key words	High-Performance Computing, Statistical Mechanics, Molecular simulation, Monte Carlo, Molecular Dynamics, Clathrate Hydrates, Phase Equilibria, Interfacial properties, Homogeneous Nucleation		

### A.2. Education

PhD, Licensed, Graduate	University	Year
Physics	Universidad de Sevilla	1992
Doctor in Chemical Engineering	Universitat Rovira i Virgili	2000

### A.3. General indicators of quality of scientific production (see instructions)

- 4 research periods recognized (1996-2001, 2002-2007, 2008-2013, 2014-2019).
- 5 teaching periods recognized (1996-2000, 2001-2005, 2006-2010, 2011-2015, 2016-2020).
- 4 PhD thesis supervised in 10 years (+ 2 more PhD thesis in course).
- ~4800 cites in Google Scholar (GS).
- Averages cites in last five years (including 2019): ~320/year (GS).
- Averages of cites/publications: ~50 cites (GS).
- h index =37 (GS).
- Total international publications: ~100. Publications in Q1: 86 (88%).
- 11 publications with more than 100 cites (1 with 500 and 2 with more than 300).

### Part B. CV SUMMARY (max. 3500 characters, including spaces)

Felipe J. Blas received a B. Sc. (Licenciatura) in Physics (Univ. of Seville, 1992) and a PhD in Chemical Engineering (Univ. Rovira i Virgili, 2000, Extraordinary PhD Award) under the supervision of Dr. Lourdes F. Vega. As a Postdoctoral Research Associate, he joined Prof. George Jackson's group at Department of Chemical Engineering, Imperial College London (UK, 2000 and 2001). He started an appointment as Assistant Professor at the Universidad de Huelva (Spain). Dr. Blas has done several predoctoral (Cornell University, 1996 and 1997) and postdoctoral (Superior Technical Institute of Lisbon and Complex Fluids Laboratory of Université of Pau – CNRS, France) stays. At the end of 2009, he became principal investigator of his research group in Huelva. In 2017, he received the 2016 AIQBE Prize in the Scientific Technical Area corresponding to the 2016 Cátedra AIQBE Award (Association of Chemical, Basics and Energetic Industries of Huelva) from University of Huelva, an award in recognition of his research activity in this area. He has been promoted several times, including Associate Professor in Applied Physics (2004) and ANECA accreditation for Professor (2013), until the current position of Full Professor in Applied Physics (2017). He is an expert in the application, development, and extension of Statistical Thermodynamic theories for the prediction of thermodynamic properties and phase equilibria of complex mixtures of industrial interest. He has large experience in the use and development of density functionals and density gradient theory, based on perturbation theories, for the prediction of interfacial properties of complex mixtures, including hydrocarbons, water, amines, CO<sub>2</sub>, etc. He has developed and applied Monte Carlo

simulation and Molecular Dynamics simulation methods during last fifteen years for the determination of thermodynamic, structural, and dynamical properties, as well as phase equilibria and interfacial properties of complex systems. During last year, he has moved towards the study of phase equilibria of clathrate hydrates of natural gases, such as CO<sub>2</sub>, CH<sub>4</sub>, and THF. Dr. Blas is co-author of more than 100 papers in JCR international journals, with near 90% of the manuscripts in Q1 and he has presented more than 150 contributions in national and international scientific conferences, including invited talks in the Royal Society of Chemistry, IUPAC Conferences on Chemical Thermodynamics and Simposia on Thermophysical Properties at Boulder (USA). He has been involved in more than 30 research projects and industrial contracts as participant and principal investigator. He has participated in 6 research contracts with industry, two in UK and four in Spain (Huelva). Dr. Blas collaborates with many research groups (Complutense Univ., Vigo Univ., CSIC, Imperial College London, Technical Univ. of Lisbon, Université de Pau et des Pays de l'Adour, Vanderbilt University, USA, and Concepción Univ., Chile). Much of the collaborators are part of the Spanish Molecular Simulation Network. The Network is coordinated by him since its creation in 2011 and it has been funding by three different Excellence Networks research projects from Spanish Government. He is the Coordinator and Director of the **Official Master in Molecular Simulation** of University of Huelva and Andalusian International University since 2018.

### **Part C. RELEVANT MERITS** (*sorted by typology*)

#### **C.1. Publications** (*see instructions*)

- I. M. Zerón, J. Algaba, J. M. Míguez, B. Mendiboure, and F. J. Blas, **Rotationally invariant local bond order parameters for accurate determination of hydrate structures**, Mol. Phys. e2395438 (2024).
- M. J. Torrejón, C. Romero-Guzmán, M. M. Piñeiro, F. J. Blas, and J. Algaba, **Simulation of the THF hydrate–water interfacial free energy from computer simulation**, J. Chem. Phys. **161**, 064701 (2024).
- M.J. Torrejón, J. Algaba, and F. J. Blas, **Dissociation line and driving force for nucleation of the nitrogen hydrate from computer simulation. II. Effect of multiple occupancy**, J. Chem. Phys. **161**, 054712 (2024).
- J. Algaba, S. Blazquez, J. M. Míguez, M. M. Conde, and F. J. Blas, **Three-phase equilibria of hydrates from computer simulation. III. Effect of dispersive interactions in the methane and carbon dioxide hydrate**, J. Chem. Phys. **160**, 164723 (2024).
- J. Algaba, S. Blazquez, E. Fera, J. M. Míguez, M. M. Conde, and F. J. Blas, **Three-phase equilibria of hydrates from computer simulation. II. Finite-size effects in the carbon dioxide hydrate**, J. Chem. Phys. **160**, 164722 (2024).
- S. Blazquez, J. Algaba, J. M. Míguez, C. Vega, F. J. Blas, and M. M. Conde, **Three-phase equilibria of hydrates from computer simulation. I. Finite-size effects in the methane hydrate**, J. Chem. Phys. **160**, 164721 (2024).
- J. Algaba, C. Romero-Guzmán, M. J. Torrejón, and F. J. Blas, **Prediction of the univariant two-phase coexistence line of the tetrahydrofuran hydrate from computer simulation**, J. Chem. Phys. **160**, 164718 (2024).
- A. R. Tejedor, I. Sanchez-Burgos, E. Sanz, C. Vega, F. J. Blas, R. L. Davidchack, N. Di Pasquale, J. Ramirez, and J. R. Espinosa, **Mold: a LAMMPS package to compute interfacial free energies and nucleation rates**, Journal of Open Source Software **9**, 6083 (2024).
- I. M. Zerón, M. Cueto Mora, and F. J. Blas, **Transport properties of the square-well fluid from molecular dynamics simulation**, Mol. Phys. e2302385 (2024).
- J. Algaba, M. J. Torrejón, and F. J. Blas, **Dissociation line and driving force for nucleation of the nitrogen hydrate from computer simulation**, J. Chem. Phys. **159**, 224707 (2023).
- F. Sastre and F. J. Blas, **Molecular simulation of the vapour-liquid coexistence curve of square-well dimer fluids**, Mol. Phys. e2238092 (2023).

- J. Algaba, A. Morales-Aragon, C. Romero-Guzmán, P. Gómez-Álvarez, and F. J. Blas, **Interfacial properties of square-well chains from molecular dynamics simulation**, Mol. Phys. **e2195022** (2023),
- C. Romero-Guzmán, I. M. Zerón, J. Algaba, B. Mendiboure, J. M. Míguez, and F. J. Blas, **Effect of pressure on the carbon dioxide hydrate – water interfacial free energy along its dissociation line**, J. Chem. Phys. **158**, 194794 (2023).
- J. Algaba, I. M. Zerón, J. M. Míguez, J. Grabowska, S. Blazquez, E. Sanz, CV. Vega, and F. J. Blas, **Solubility of carbon dioxide in water: Some useful results for hydrate nucleation**, J. Chem. Phys. **158**, 184703 (2023).

### **C.2. Research projects**

- Title: **Entendiendo la nucleación de hidratos de hidrógeno desde una perspectiva molecular (NUCLEA-H2) (EPIT-1282023)**

Financing institution: Programa Operativo FEDER Andalucía 2021-2027 – Univ. de Huelva

Dates, since: 25-05-2024 until: 24-05-2027. Funding: 73,100 €

Type of participation: Principal Investigator

- Title: **Equilibrio de fase, nucleación y propiedades dinámicas de hidratos y clatratos mediante técnicas avanzadas de simulación molecular (PDI-2021-125081NB-I00)**

Financing institution: Ministerio de Ciencia e Innovación

Dates, since: 01-09-2022 until: 30-08-2025. Funding: 90,750 € + 1 FPI contract

- Title: **Equilibrio de fase de hidratos de metano y dióxido de carbono en presencia de promotores termodinámicos y cinéticos (UHU-202034)**

Financing institution: Programa Operativo FEDER Andalucía 2014-2020 – Univ. de Huelva

Dates, since: 01-01-2022 until: 30-06-2023. Funding: 40,000 €

- Title: **Nucleación de hidratos de metano y dióxido de carbono (P20-00363)**

Financing institution: Junta de Andalucía

Dates, since: 23-06-2020 until: 31-12-2022. Funding: 73,650 €

Type of participation: Principal Investigator

- Title: **Estudio de los parámetros termodinámicos y cinéticos en la transición sólido-líquido de clatratos, hidratos de metano y dióxido de carbono (UHU-1255522)**

Financing institution: Programa Operativo FEDER Andalucía 2014-2020 – Univ. de Huelva

Dates, since: 01-01-2020 until: 31-12-2022. Funding: 39,797 €

- Title: **Red de Simulación Molecular (RED2018-102593-T)**

Financing institution: Ministerio de Economía y Competitividad

Dates, since: 01-01-2020 until: 31-12-2022. Funding: 15,000 €

Type of participation: Principal Investigator

- Title: **Autoensamblado y sistemas estructurados en redes (FIS2017-89361-C3-1-P)**

Financing institution: Ministerio de Economía, Industria y Competitividad

Dates, since: 01-01-2018 until: 30-09-2021 (extended 9 months), Funding: 54,450 €

Type of participation: Principal Investigator of the coordinated research project and the subproject of University of Huelva

- Title: **Red de Simulación Molecular (FIS2015-71749-REDT)**

Financing institution: Ministerio de Economía y Competitividad

Dates, since: 01-12-2015 until: 01-12-2018. Funding: 30,000 €

Type of participation: Principal Investigator

- Title: **Fluctuaciones en interfases: campos externos y gradientes de composición (FIS2013-46920-C2-1-P)**

Financing institution: Ministerio de Economía y Competitividad

Dates, since: 01-01-2014 until: 31-12-2017. Funding: 30,000 €

Type of participation: Principal Investigator

### **C.3. Contracts, technological or transfer merits**

- **Modelling of interfaces and phases of water-oil-surfactant systems in squeeze treatments of oil fields (GR/N20317/01)**

Financing institution/industry: EPSRC and BP Exploration Ltd

Dates, since: July 2001 until: October 2002. Funding: 137,809€

Tipo de participación: Investigador

- **Estudio de los factores físico-químicos que controlan las pérdidas de Cu en los procesos de fusión flash (Ref. 10/2014)**

Financing institution/industry: Atlantic Copper SLU

Dates, since: January 2014 until: November 2014. Funding: 35,000€

Tipo de participación: Investigador

- **Estudio de los factores físico-químicos que controlan las pérdidas de Cu en los procesos de fusión flash. Segundo año (Ref. 7/2015)**

Financing institution/industry: Atlantic Copper SLU

Dates, since: November 2014 until: February 2016. Funding: 84,715€

Tipo de participación: Investigador

- **Estudio físico-químico de las escorias y mata de los hornos flash y eléctrico enfocado al análisis de las pérdidas de cobre (Ref. 29/2016)**

Financing institution/industry: Atlantic Copper SLU

Dates, since: June 2016 until: January 2018. Funding: 91,900€

Tipo de participación: Investigador

**C.5 Research visits in other Research Centres:**

- Olin Hall, Chemical Engineering, Cornell University, Ithaca (NY), USA. Dates: September-December 1996, Duration (weeks): 16; November - December 1997 Duration (weeks): 5

- Department of Chemical Engineering and Chemical Technology, Imperial College London, London, Reino Unido Dates: July 2000 – March 2001 Duration (weeks): 40

- Centro de Química Estructural, Instituto Superior Técnico, Universidade Técnica de Lisboa, Lisboa, Portugal Dates: June-July 2007 Duration (weeks): 8

- Laboratoire des Fluides Complexes et Leurs Reservoirs, UMR5051 (Unidad Mixta de Investigación), Université de Pau et des Pays de l'Adour, CNRS y TOTAL S.A., Francia Dates: June-July 2013 Duration (weeks): 5

**C.6 Teaching (during the last 6 years):**

- Physics (First-year course, Chemistry Degree, 6 ECTS), between 2019-20 and 2024-25.

- Physical Chemical Basis of Statistical Mechanics (Course in Molecular Simulation Master Degree, 2 ECTS), between 2019-20 and 2024-2025.

- Physical Chemical Basis of Thermodynamics (Course in Molecular Simulation Master Degree, 3 ECTS), between 2021-22 and 2024-2025.

**C.7 ... Others**

- AIQBE Award Investigación del Área Científico Tecnológica 2016, Cátedra AIQBE (Asociación de Industrias Químicas, Básicas y Energéticas) de la Universidad de Huelva.

- Vice Rector of Research and Transfer of University of Huelva (13/11/2015 - 31/03/2016).

- Associate Dean of Postgraduate of the Faculty of Experimental Sciences, University of Huelva (6/10/2017 – 2/7/2020).

- Head of the Department of Integrated Sciences (Physics, Mathematics, and Biology) of University of Huelva (3/7/2020 – 8/10/2021).

- Director of the Theoretical Physics and Mathematics Research Center of University of Huelva (01/02/2012 - 31/07/2015).

- Research Grant Reviewer: (1) ANEP (ANEP Areas: Physics and Space Sciences and Science and Technology of Materials). (2) Andalusian Agency of Evaluation of Quality and Accreditation (AGAE). (3) Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR).

- National Coordinator of the Spanish Molecular Simulation Network (since 2011). Chairman of 3 Schools and 9 National Workshops of the Spanish Molecular Simulation Network.

- Chairman and organizer of the **VI Reunión Nacional de Física Estadística (FISES'09)** of the RSEF y **XV Encuentro Inter-Bienal del Grupo Especializado de Termodinámica (GET)** of the RSEF y ESQE, Huelva (september 2009 and september 2016).

- Coordinator and Director of the **Official Master in Molecular Simulation** of University of Huelva and Andalusian International University (**Official Title Code: 4316581**. Beginning course: 2018-2019).

- Chairman and organizer of the International Congress: **26th Bienial Thermodynamics Conference, Thermodynamics'2019** of the Royal Society of Chemistry (Punta Umbria, Huelva, 26-28 June, 2019).

- Guest Editor of the Special Issue Thermodynamics'2019 of **Molecular Physics** (2020).