

**Part A. PERSONAL INFORMATION**

CV date

13/06/2022

First and Family name	Felipe Jiménez Blas		
Social Security, Passport, ID number	29481367J	Age	52
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	From	19/10/2017
Key words	High-Performance Computing, Statistical Mechanics, Molecular simulation, Monte Carlo, Molecular Dynamics, Complex fluids, Interfaces, Clathrate Hydrates		

**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.
- 4173 cites in Google Scholar (GS).
- Averages cites in last five years (including 2021): 270/year (GS).
- Averages of cites/publications: 50 cites (GS).
- h index =36 (GS).
- Total international publications: 89 publications in Q1: 78 (88%).
- 8 publications with more than 100 cites (1 with more than 400 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 80 papers in JCR international journals, with near 90% of the manuscripts in Q1 and he has presented more than 100 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)

- J. Algaba, E. Acuña-Yeomans, J. M. Míguez, B. Mendiboure, and F. J. Blas, **Simulation of the carbon dioxide hydrate – water interfacial energy**, *J. Colloid & Interface Sci.* 623, 354 (2022).
- E. Feria, J. Algaba, J. M. Míguez, A. Mejía, and F. J. Blas, **Molecular dynamics of liquid-liquid equilibrium and interfacial properties of aqueous solutions of methyl esters**, *Phys. Chem. Chem. Phys.* 24, 5371 (2022).
- A. Mejía, M. Cartes, G. Chaparro, E. Feria, F. J. Blas, J. M. Míguez, J. Algaba, and E. A. Müller, **Phase equilibria and interfacial properties of selected methane + n-alkane binary mixtures**, *J. Mol. Liquids* 34, 116918 (2021).
- J. Algaba, J. M. Míguez, P. Gómez-Álvarez, A. Mejía and F. J. Blas, **Preferential Orientations and Anomalous Interfacial Tensions in Aqueous Solutions of Alcohols**, *J. Phys. Chem. B* 124, 8388 (2020).
- J. Algaba, M. Cartes, A. Mejía, J. M. Míguez, and F. J. Blas, **Phase equilibria and interfacial properties of the tetrahydrofurane + methane binary mixture from experiment and computer simulation**, *Journal of Physical Chemistry C* 123, 20960 (2019).
- J. Algaba, J. M. Garrido, J. M. Míguez, A. Mejía, A. I. Ignacio Moreno-Ventas Bravo, and F. J. Blas, **Interfacial properties of tetrahydrofurane and carbon dioxide mixture from computer simulation**, *Journal of Physical Chemistry C* 122, 16142 (2018).
- M. Pérez-Rodríguez, A. Vidal-Vidal, J. M. Míguez, F. J. Blas, J.-P. Torr , and M. M. Pi eiro, **Computational study of the interplay between intermolecular interactions and CO<sub>2</sub> orientations in type I hydrates**, *Physical Chemistry Chemical Physics* 19, 3384 (2017).
- J. M. Garrido, J. Alaba, J. M. Míguez, B. Mendiboure, A. I. Moreno-Ventas Bravo, M. M. Pi eiro, and J. Algaba, **On interfacial properties of tetrahydrofurane: atomistic and coarse-grained models from molecular dynamics simulation**, *Journal of Chemical Physics* 144, 144702 (2016).
- J. M. Míguez, M. M. Conde, J.-P. Torr , F. J. Blas, M. M. Pi eiro, and C. Vega, **Molecular dynamics simulation of CO<sub>2</sub> hydrates: prediction of three phase coexistence line**, *Journal of Chemical Physics* 142, 124505 (2015).

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

- Title: **Equilibrio de fase de hidratos de metano y di ido de carbono en presencia de promotores termodin micos y cin ticos (UHU-202034)**

Financing institution: Programa Operativo FEDER Andaluc a 2014-2020 – Univ. de Huelva  
Dates, since: 01-01-2022 until: 30-06-2023. Funding: 40,000 €

- Title: **Nucleaci n de hidratos de metano y di ido de carbono (P20-00363)**

Financing institution: Junta de Andaluc a

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 interfaces: 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
  - Title: **Red de Simulación Molecular (RdSiMol) (FIS2011-13119-E)**  
Financing institution: Ministerio de Ciencia e Innovación, Subprograma de Acciones Complementarias  
Dates, since: 01-01-2012 until: 30-06-2013. Funding: 15,000 €  
Type of participation: Principal Investigator
  - Title: **Teoría y simulación de propiedades interfaciales y equilibrio de fases de fluidos complejos (FIS2010-14866)**  
Financing institution: Ministerio de Ciencia e Innovación  
Dates, since: 01-01-2011 until: 31-12-2014. Funding: 43,560 €  
Type of participation: Principal Investigator
  - Title: **Comparative study between models and experiments of CO<sub>2</sub> adsorption on porous media (FR2009-0056)**  
Financing institution: Ministerio de Ciencia e Innovación, Subprograma de Acciones Integradas  
Dates, since: 01-01-2010 until: 30-06-2013. Funding: 11,000 €  
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
  - **Modelling thermodynamics for oil extraction (CA019004282)**  
Financing institution/industry: BP Amoco Exploration  
Dates, since: June 2000 until: June 2003. Funding: 97,830€  
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, C.7 ... Others**

- Extraordinary Doctorate Award, Universitat Rovira i Virgili, 2000-2001.

- 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 Postgrade 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).

- PhD Thesis: Francisco José Martínez Ruiz, "**Propiedades interfaciales y de equilibrio de fase de mezclas fluidas mediante simulación Monte Carlo**", Sobresaliente cum laude por unanimidad (European PhD), November 2015, University of Huelva.

- PhD Thesis: Jesús Algaba Fernández, "**Propiedades estructurales y equilibrio de fase de promotores/inhibidores de hidratos mediante simulación molecular**", Sobresaliente cum laude por unanimidad (European PHD), September 2019, University of Huelva.

- PhD Thesis: Esther Feria Delgado, "**Equilibrio de fase y propiedades interfaciales de cadenas moleculares de interés industrial mediante simulación molecular**", PhD defense will be in May 2022, University of Huelva.

- Member of the *Editorial Advisory Board of the Journal of Chemical and Engineering Data (American Chemical Society)* (2015-2020).

- 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 6 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 **Oficial 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 Bienal Thermodynamics Conference, Thermodynamics'2019** of the Royal Society of Chemistry (Punta Umbría, Huelva, 26-28 June, 2019).

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

- 3 funded infrastructure research projects from Ministerio de Ciencia (**UNUH15-CE-2930, EQ2019-006073-P**) and Junta de Andalucía (**5223(1150740)**) for computational resources for our research group: **40.000 €** in 2016, **45.000 €** in 2017, and **100.000 €** in 2019.