José Ortega Mateo

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Professional Preparation:

Undergraduate:	UAM	Physics	1981-1986
Graduate:	UAM	Physics, Ph.D.	1986-1991
Postdoctoral:	Arizona State University (USA)		1992-1993
Postdoctoral:	University of Cambridge (UK)		1993-1994

Professional Appointments:

2017-present	Catedrático de Universidad (Professor), UAM
1995-2017	Profesor Titular de Universidad (Associate Professor), UAM

Research Lines:

Computational studies of biomolecular materials: QM/MM simulations in biomolecules. Enzymatic reactions. Ultrafast photochemical processes in biomolecules. Proton transfer in peptide nanotubes.

Development of efficient first-principles techniques for the simulation of complex materials: Local-orbital Density Functional Theory (DFT) methods (FIREBALL code). Non-adiabatic Molecular-Dynamics. Quantum Mechanics/Molecular Mechanics (QM/MM) approach. Theoretical simulation of Scanning Tunneling Microscope (STM).

Atomic, electronic and dynamic properties of semiconductor surfaces. Structural and metal/insulator transitions in clean and metal decorated semiconductor surfaces. Electron correlation effects. Metal/semiconductor Interfaces.

Interfaces of Organic Semiconductors: The Molecule/Metal Interface. Metal/Organic, Organic/Organic and Organic/Inorganic interfaces. Energy level alignment.

Citation Metrics

Total number of publications in SCI journals: 138.

Number of citations: 4736. H-index: 37

Source: *Web of Science* (Date: 11/2021)

Recent Research Projects

1.- Reference: PID2021-125604NB-I00. *Computational Studies of Biomolecular and Bioinspired Materials.* PIs: José Ortega Mateo (UAM) and Linda A. Zotti (UAM). Ministry of Science and Innovation (Spain), 09/2022 --08/2025. 108.900 €.

2.- Reference: MAT2017-88258-R. *Modelling of Complex Materials: Biomolecules and Two-dimensional systems.* PIs: José Ortega Mateo (UAM) and Blanca Biel Ruiz (UGR). Ministry of Science and Innovation (Spain), 01/2018--12/2021. 121.000 €.

3.- Reference: MAT2014-59966R. *Materials modelling at the Nanoscale*. PIs: José Ortega Mateo (UAM) and Fernando Flores Sintas (UAM). Ministry of Science and Innovation (Spain), 01/2015--12/2017. 157.300 €.

5 Selected Recent Publications

Coupled Sublattice Melting and Charge-Order Transition in Two Dimensions. T. S. Smith, F. Ming, D. G. Trabada, C. Gonzalez, D. Soler-Polo, F. Flores, J. Ortega, and H. H. Weitering. PHYSICAL REVIEW LETTERS 124, 097602 (2020).

Proton Transfer in Guanine-Cytosine Base Pairs in B-DNA. D. Soler-Polo, J.I. Mendieta-Moreno, D. G. Trabada, J. Mendieta and J. Ortega, JOURNAL OF CHEMICAL THEORY AND COMPUTATION 15, 6984 (2019).

DFT molecular dynamics and free energy analysis of a charge density wave surface system. D. G. Trabada, J.I. Mendieta-Moreno, D. Soler-Polo, F. Flores, J. Ortega. APPLIED SURFACE SCIENCE 479, 260-264 (2019).

Adsorption Geometry and Energy Level Alignment at the PTCDA/TiO2(110) Interface. Sylvie Rangan, Charles Ruggieri, Robert Bartynski, José Ignacio Martínez, Fernando Flores, and José Ortega. THE JOURNAL OF PHYSICAL CHEMISTRY B 122, 534-42 (2018).

Quantum Mechanics/Molecular Mechanics Free Energy Maps and Nonadiabatic Simulations for a Photochemical Reaction in DNA: Cyclobutane Thymine Dimer. J.I. Mendieta-Moreno, D.G. Trabada, J. Mendieta, J.P. Lewis, P.Gómez-Puertas, J.Ortega. THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS 7, 4391-4397 (2016).

Thesis Advisor of: M.A. Basanta, C. González, D.G. Trabada, E. Abad, J.I. Mendieta, Diego Soler-Polo, Jorge Vega (current Ph.D. student).

Postgraduate-Scholar Advisor of: Barbara Pieczyrak, Juan I. Beltrán, José I. Martínez, Yannick J. Dappe, Pavel Jelínek.

Graduate Advisor: Fernando Flores (Universidad Autónoma de Madrid)

Postdoctoral Advisors: Volker Heine—University of Cambridge
Otto F. Sankey—Arizona State University