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Professor in Chemical Physics

PhD. Universidad Complutense de Madrid, 1975.

Postdoctoral Associate, Yale University, 1975-77.

Associate Professor/Professor, Universidad Complutense, 1978-2004.

Since 2004 in “Universidad Nacional de Educación a Distancia” Madrid, Spain.

Research Projects

Coordinator of 8 National Projects (Spanish Ministry for Research) and Spanish Coordinator of 2 Network Projects from European Frames.

Some recent publications

- "Conformational Properties of Branched Polymers: Theory and Simulations" J. J. Freire. Adv. Polym. Sci. 143, 35 (1999).
- "Determination of Potential Parameters for Alkanes" A. Lopez Rodriguez, C. Vega and J. J. Freire. J. Chem. Phys. 111, 438 (1999).
- "Conformational Properties of Polymer Chains in the Theta Region" A. M. Rubio, J. J. Freire, C. W. Yong and J. H. R. Clarke. J. Chem. Phys. 111, 1302 (1999).
- "Interaction between Two Star Chains in a Good Solvent" A. M. Rubio and J. J. Freire. Comp. and Theor. Polymer Science, 10, 89 (2000).
- "Phase Separation of Binary Homopolymer and Ternary Homopolymer-Copolymer Mixtures through Gibbs Ensemble Simulations" A. Poncela, A. M. Rubio and J. J. Freire. J. Chem. Phys. 114, 8174 (2001).
- "Form Factor of an Isolated Chain with Excluded Volume" J. J. Freire, G. Alvarez and M. Bishop. Macromol. Theory Simul. 11, 11 (2002).
- "Dynamics of Bond Fluctuation Model Chains in Good and Theta Solvents" A. M. Rubio, M. Storey, J. F. M. Lodge and J. J. Freire. Macromol. Theory Simul. 11, 171 (2002).
- "Monte Carlo Simulation of Star Polymer Systems with the Bond Fluctuation Model" A. Di Cecca and J. J. Freire. Macromolecules, 35, 2851 (2002).
- "Cyclization Kinetics of Nondiluted Bond Fluctuation Chains" A. M. Rubio, M. Pita and J. J. Freire. Macromolecules, 35, 5681 (2002).

- "Mesophase Formation in Solutions of Diblock Copolymers Simulated Using the Bond Fluctuation Model" J. J. Freire and C. McBride. *Macromol. Theory Simul.* 12, 237 (2003).
- "Simulation Results for the Size and Intrinsic Viscosity of Several Dendrimer Molecules" J. J. Freire, E. Rodríguez and A. M. Rubio, *J. Chem. Phys.* 123, 154901 (2005).
- "Effects of the Chain Architecture on the Miscibility of Symmetric Linear/Linear and Star/Star Polymer Blends" P. E. Theodorakis, A. Avgeropoulos, J. J. Freire, M. Kosmas, and C. Vlahos, *Macromolecules* 39, 4235 (2006).
- "Polyfunctional MDI oligomers through dendrimerization" M. Martinelli, M. Calderón, E. Rodríguez, J. J. Freire and M. C. Strumia, *Eur. Polym. J.* 43, 1978 (2007).
- "Intramolecular Distances and Form Factor of Cyclic Chains with Excluded Volume Interactions" A. M. Rubio, G. Álvarez and J. J. Freire, *Polymer*, 49, 628 (2008).
- "Conformational Properties and Rouse Dynamics of Different Dendrimer Molecules" J.J. Freire and A. M. Rubio, *Polymer*, 49, 2762 (2008).
- "Influence of Chain Topology and Bond Potential on the Glass Transition of Polymer Chains Simulated with the Bond Fluctuation Model" J. J. Freire, *J. Phys.: Condens. Matter* 20, 285102 (2008).
- "Realistic Numerical Simulations of Dendrimer Molecules" J. J. Freire, *Soft Matter* 4, 2139 (2008).
- "Coarse-Grained Model for Polybenzylether Dendritic Molecules" J. J. Freire, *Soft Matter* 5, 1912 (2009).
- "Molecular dynamics simulation of miscibility in several polymer blends" A. Ahmadi and J. J. Freire, *Polymer*, 50, 4973 (2009).
- "Forcefield parameterization and molecular dynamics simulation of flexible POSSlinked (NHC) (phosphine) Ru catalytic complexes" A. Ahmadi, C. McBride, J. J. Freire, A. Kajetanowicz, J. Czaban and K. Grela, *J. Phys. Chem. A*, 115, 12017 (2011).
- "Dielectric and molecular dynamics study of the secondary relaxations of poly(styrene-co-methylmethacrylate) copolymers: Influence of the molecular architecture" M. Encinar, M.G. Prolongo, R.G. Rubio, F. Ortega, A. Ahmadi, and J.J. Freire, *Eur. Phys. J.* 34, 134 (2011).
- "Molecular dynamics simulations of the protonated G4 PAMAM dendrimer in an ionic liquid system" J.J. Freire, A. Ahmadi, and C. McBride, *J. Phys. Chem. B*, 117, 15157 (2013).
- "Simulation study of the G=4 PAMAM dendrimer in water at different pH conditions" J.J. Freire, P. Efthymiopoulos and A. Ahmadi, *Per. Pol. Chem. Eng.*, 58, 49 (2014).

"Binary Interactions between Dendrimer Molecules. A Simulation Study" A. M. Rubio, C. McBride and J.J. Freire, *Macromolecules*, 47, 5379 (2014).

"Coarse-Grained and Atomistic Simulations for the G=4 PAMAM-EDA Dendrimer" J.J. Freire, A. M. Rubio and C. McBride, *Macromol. Theor. Simul.*, 24, 432 (2015).

Citation report (from I.S.I., Web of Science; ResearcherID: J-2287-2014)

Total number of citations: 2188.

5 most cited articles:

"Theory of DNA Melting Curves" [Fixman M](#), Freire [JJ](#), *Biopolymers* 16 (12): 2693-2704, 1977. 188 citations.

"Conformational Properties of Branched Polymers: Theory and Simulations" J. J. Freire. *Adv. Polym. Sci.* 143, 35 (1999). 109 citations.

"Monte-Carlo Calculation of Hydrodynamic Properties of Freely Jointed, Freely Rotating, and Real Polymethylene Chains", [de La Torre JG](#), [Jimenez A](#), [Freire JJ](#), *Macromolecules* 15 (1): 148-154, 1982. 94 citations.

"Monte-Carlo Calculations for Linear-Chains and Star Polymers with Intramolecular Interactions .3. Dimensions and Hydrodynamic Properties In Good Solvent Conditions" [Rey A](#), [Freire JJ](#), [de La Torre JG](#), *Macromolecules* 20 (2): 342-346, 1987. 86 citations.

"Monte-Carlo Calculations for Linear and Star Polymers with Intramolecular Interactions .1. Dimensions" [Freire JJ](#), [Pla J](#), [Rey A](#), [Prats R](#), *Macromolecules* 19 (2): 452-457, 1986. 76 citations.

h factor: 24.

In the list "Most Cited Chemists, 1983-1997", based in Science Citation Index

<http://ftp.ccp14.ac.uk/ccp/web-mirrors/armel/www.cristal.org/chimie/chimistes.html>

In the list of "important Spanish Researchers"

<http://indice-h.webcindario.com/>

("Tecnología, Ingeniería y Ciencias Aplicadas"/"Ciencia de los Materiales"/"Polymer Science").

In the list of "Top Reviewers JCP 2014"

http://friedel.uned.es/juan/top_reviewers_2014.pdf

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