GUADALUPE JIMÉNEZ-SERRATOS

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RESEARCH INTERESTS

- Molecular simulations of fluids to understand and predict thermodynamic properties in complex systems.
- Development of coarse-grained (CG) molecular models with realistic behaviour to bridge computational simulations and experimental results.

Molecular Dynamics simulation · Monte Carlo simulations · Coarse-grained models
Asphaltene aggregation · Liquid crystals · Self-assembling systems · Polymers
Confined systems · SAFT Equation of State · Phase diagrams

Currently working on the EPSRC-NSF joint grant "Molecular Engineering of Inhibitors to Self-Assembly: Fundamental structure informing in silico design", led by Prof. Erich A. Müller (Imperial College London, U.K.), Dr. Thomas F. Headen (STFC Rutherford Appleton Laboratory, U.K.), and Dr. Michael P. Hoepfner (University of Utah, U.S.A.). Previously, part of the BP-ICAM15 (2015-2018) http://www.icam-online.org/research and UNIHEAT (2013-2015) http://www.uniheat-project.com projects, both focused on the study of asphaltene aggregation an deposition problems.

EXPERIENCE

- 2013-Present. **Research Associate**.
  Department of Chemical Engineering, Imperial College London, U.K.
  Line managers: Prof. Erich A. Müller and Prof. George Jackson.
- 2017, 2018. **Consultant for ConocoPhillips**.
  Led by Prof. Erich A. Müller. Imperial College London.
- 2008. **Technician** at the Quantum Applications and Nanophotonics Laboratory.
  Physics Institute of the University of Guanajuato (Leon, Mexico).
  Line manager: Prof. José Luis Lucio Martínez.

EDUCATION

- 2009-2013. **PhD. in Physics**.
  Thesis: *Primitive models of self-assembling systems using discontinuous and long-range potentials.*
  Thesis advisor: Prof. Alejandro Gil Villegas Montiel. University of Guanajuato, Mexico.
- 2006-2008. **Masters in Science (Physics)**.
  Thesis: *Dynamic light scattering (DLS) in worm-like micelles.*
  Thesis advisor: Prof. Rolando Crisóstomo Castillo Caballero. National Autonomous University of Mexico, Mexico.
- 2000-2005. **B.Sc. in Physics Engineering**.
  Thesis: *Modelling of calorific properties for asphaltene primitive models.*
  Thesis advisor: Prof. Alejandro Gil Villegas Montiel. University of Guanajuato, Mexico.

SKILLS

- Programming skills (Fortran)
- Monte Carlo simulations (experience in home-made codes)
- Molecular Dynamics simulation software (GROMACS, HOOMD-blue)
- Development of coarse-grained models with Mie force fields obtained via the Statistical Associating Fluid Theory equation of state
- Communication and time-management skills developed from the experience in interdisciplinary and industrial research projects.
- Scientific tools (Grace, LaTeX, VMD, Origin, etc.).

TEACHING

- Support and training to PhD students of the MSE group (2013-present).
- Thermodynamics 1 (CE1-05) 2014-2015 and 2015-2016. Teaching Assistant. Imperial College London.

AWARDS AND MEMBERSHIPS

- AIChE member, Postdoctoral researcher (2018).
- Member of the Mexican Soft Condensed Matter Network (2018).
- **National Researchers System (SNI) Level 1 (Mexico 2015)**.
- Academic Trajectory Award, PhD in Physics, University of Guanajuato, Mexico (2013).
- PhD Laureate thesis award (Mexico 2013).
- BPhys Laureate thesis award (Mexico 2005).

INTERNSHIPS

- **Primitive models of self-assembling systems with discontinuous potentials.**
  Under the "Beca Mixta CONACyT" program (scholarship)
  Advisor: Prof. Carlos Vega de las Heras. Department of Physical Chemistry, Universidad Complutense de Madrid. Madrid, Spain (Feb-Nov 2011).
- $Si(111)\sqrt{3}\times\sqrt{3}$ **surface second-harmonic generation.**
  Professional service
  Advisor: Prof. Bernardo Mendoza Santoyo. Center for Research in Optics. Leon, Mexico (Feb-Nov 2005).

CONFERENCES AND SEMINARS

- **2018 AIChE Annual Meeting**. Pittsburgh, USA (27^{th} October-2^{nd} November 2018). Oral presentation.
- **Frontiers of Molecular Engineering**. Chicago, USA (26^{th}-30^{th} September 2018). Poster presentation.
- **Thermodynamics 2017**. Edinburgh, UK (5^{th}-8^{th} September 2017). Poster presentation
- **Petrophase 2017.** Le Havre, France (11^{th}-15^{th} June 2017). Poster presentation
- 14^{th} **International Conference on Properties and Phase Equilibria for Product and Process Design.** Porto, Portugal (22^{nd}-26^{th} May 2016). Poster presentation.
- **Petrophase 2016.** Elsinore, Denmark (19^{th}-23^{rd} June 2016). Poster presentation.
- **Thermodynamics 2015**. Copenhagen, Denmark (15^{th}-18^{th} September 2015).
- **UNIHEAT - Energy efficient heat exchange and catalysis Joint Workshop.** Boreskov Institute of Catalysis. Novosibirsk, Russia (April 2015) · Imperial College London. London, UK (March 2015) · St. Petersburg, Russia (October, 2014) · Imperial College London. London, UK (March 2014). Oral presentations.
- $\mathbf{2}^{nd}$ **Meeting of the Mexican Soft Condensed Matter Network.** Guanajuato, Mexico (January 2013). Oral presentation.
- **UCM Spring Meetings.** Madrid, Spain (April 2011). Oral presentation.
- **XXXIX Winter Meeting on Statistical Physics.** Taxco, Mexico (January 2010). Poster presentation.
- **XXXVII Winter Meeting on Statistical Physics.** Taxco, Mexico (January 2008). Poster presentation.

PROFESSIONAL REFERENCES

- Prof. Erich A. Müller
  Department of Chemical Engineering, Imperial College London, U.K.
  e.muller@imperial.ac.uk
- Prof. George Jackson
  Department of Chemical Engineering, Imperial College London, U.K.
  g.jackson@imperial.ac.uk
- Dr. Tim S. Totton
  Strategy Analyst at BP, BP Exploration Operating Co. Ltd., U.K.
  tim.totton@uk.bp.com

LIST OF PUBLICATIONS

13. **Solubilities of Pyrene in Organic Solvents: Comparison between Chemical Potential Calculations Using a Cavity-Based Method and Direct Coexistence Simulations**
    C.R. Wand, M. Fayaz-Torshizi, G. Jiménez-Serratos, E.A. Müller, and D. Frenkel.
    Journal of Chemical Thermodynamics B **131**, 620 (2019).
12. **Aggregation Behavior of Model Asphaltenes Revealed from Large-Scale Coarse-Grained Molecular Simulations**
    G. Jiménez-Serratos, T.S. Totton, G. Jackson, and E.A. Müller.
    Journal of Physical Chemistry B **123**, 2380 (2019).
11. **Fluid-Solid Phase Transition of n-Alkane Mixtures: Coarse-Grained Molecular Dynamics Simulations and Diffusion-Ordered Spectroscopy Nuclear Magnetic Resonance**
    S. Shahruddin, G. Jiménez-Serratos, G.J.P. Britovsek, O.K. Matar, and E.A. Müller.
    Scientific Reports **9**, 1002 (2019).
10. **SAFT-γ Force Fields for the Simulation of Molecular Fluids. 5. Hetero-Group Coarse-Grained Models of Linear Alkanes and the Importance of Intramolecular Interactions**
    S. Rahman, O. Lobanova, G. Jiménez-Serratos, C. Braga, V. Raptis, E.A. Müller, G. Jackson, and A. Galindo.
    Journal of Physical Chemistry B **122**, 9161 (2018).
9. **Group Contribution Coarse-Grained Molecular Simulations of Polystyrene Melts and Polystyrene Solutions in Alkanes Using the SAFT-γ Force Field**
    G. Jiménez-Serratos, C. Herdes, A. Haslam, G. Jackson, and E.A. Müller.
    Macromolecules **50**, 4840 (2017).
8. **raaSAFT: a Framework Enabling Coarse-Grained Molecular Dynamics Simulations Based on the SAFT-γ Mie Force Field**
    Å. Ervik, G. Jiménez-Serratos, and E.A. Müller.
    Computational Physics Communications, **212**, 161 (2017).
7. **A Multiscale Method for Simulating Fluid Interfaces Covered with Large Molecules such as Asphaltenes**
    Å. Ervik, M. O. Lysgaard, C. Herdes, G. Jiménez-Serratos, E.A. Müller, S.T. Munkejord, and B. Müller.
    Journal of Computational Physics **327**, 576 (2016).
6. **Crude Oil Fouling: Fluid Dynamics, Reactions and Phase Change**
    J. Yang, M.G.J. Serratos, D.S. Fari-Arole, E.A. Müller, and O.K. Matar.
    Procedia IUTAM **15**, 186 (2015).
5. **Modeling of Fouling from Molecular to Plant Scale in "Crude Oil Fouling. Deposit Characterization, Measurements, and Modeling"**
    F. Coletti, B.D. Crittenden, A.J. Haslam, G.F. Hewitt, G. Jackson, G. Jiménez-Serratos, S. Macchietto, O.K. Matar, E.A. Müller, D. Sileri, and J. Yang. F. Coletti and G. Hewitt, Eds.
    Book chapter. Gulf Professional Publishing (2014).
4. **Monte Carlo Simulation of Flexible Trimer: from Square-well chain to amphiphilic primitive models**
    G. Jiménez-Serratos, C. Vega, F. J. Blas and A. Gil-Villegas.
    Journal of Chemical Physics **139**, 114901 (2013).
3. **Evaluation of the Pressure Tensor and Surface Tension for Molecular Fluids with Discontinuous Potentials Using the Volume Perturbation Method**
    G. Jiménez-Serratos, C. Vega and A. Gil-Villegas.
    Journal of Chemical Physics **137**, 204104 (2012).
2. **Computer Simulation of Charged Hard Spherocylinders at Low Temperatures**
    G. Jiménez-Serratos, C. Avendaño, A. Gil-Villegas and E. González-Tovar
    Molecular Physics **109**, 27 (2011).
1. **Molecular Thermodynamics of Adsorption Using Discrete-Potential Systems**
    G. Jiménez, S. Santillán, C. Avendaño, M. Castro, and A. Gil-Villegas A.
    Oil & Gas Science and Technology, Rev. IFP **63**, 329 (2008).