Curriculum Vitae: Gabriel D. Barbosa, Ph. D.

Personal Data

Address: 1005 14th street, Unit 1C, Tuscaloosa, AL 35401.
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Education

September 2018. **Ph.D. in Chemical Engineering**, **Federal University of Rio de Janeiro** (UFRJ), Brazil
Thesis Title: "Thermodynamic modeling of confined fluids: obtaining an equation of state based on molecular simulation"
Advisors: Prof. Frederico W. Tavares (UFRJ) and Prof. Leonardo Travalloni (UFRJ). These studies were being carried out in collaboration with the Prof. Marcelo Castier (Texas A&M University at Qatar)

September 2015. **Ms. C. in Chemical Engineering**, **Federal University of Rio de Janeiro** (UFRJ), Brazil
Thesis Title: "Molecular simulation of fluid confined in porous media"
Advisors: Prof. Frederico W. Tavares (UFRJ) and Prof. Leonardo Travalloni (UFRJ). These studies were being carried out in collaboration with the Prof. Marcelo Castier (Texas A&M University at Qatar)

2013 **Undergraduate Degree in Environmental Engineering**, **State University of Southwestern Bahia**

Research Experience

Dr. Turner's Group, **University of Alabama** (UA)

2021 – Postdoctoral research; advisor: Prof. C. H. Turner (UA)

- Molecular Simulations of High-Performance Solvents and Ionic Liquids

ATOMS, **Federal University of Rio de Janeiro**

2018 – 2021 Postdoctoral research; advisor Prof. Frederico W. Tavares (UFRJ)

- Density Function Theory and Molecular Thermodynamics: thermodynamic modeling of inhomogeneous systems

2014 – 2018 Graduate research; advisors: Prof. Frederico W. Tavares (UFRJ) and Prof. Leonardo Travalloni

- Monte Carlo Method: confined fluid simulation and evaluation of structural properties
- Equation of State and Statistical Thermodynamic: obtaining an equation of state based on the generalized van der Waals theory
- Equilibrium Calculation: adsorption pure fluid and mixture using an extended equation of state for the adsorbed phase
- Density Function Theory: analysis of the structure of confined fluids

UESB, **State University of Southwestern Bahia**

2009 – 2013 Undergraduate research; advisor: Prof. Ronaldo Thibes

- Lagrangian and Hamiltonian Description of Constrained Systems: principle of least action and the Lagrange multipliers method

Scholarships

2021 – 2022 Postdoctoral Fellowship The U.S. Department of Energy

2018 – 2020 Postdoctoral Fellowship CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior), Brazil

2016 – 2018 Doctoral Fellowship CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior), Brazil.

2014 – 2016 Fellowship COPPETEC Foundation, Brazil

Publications

2023 Kolesnikov AL, Budkov YA, **Barbosa GD**, Moller J, Taveres FW. Water adsorption on planar interfaces: classical density functional study. *Fluid Phase Equilibria* **564**, 113567. (DOI)

2022 **Barbosa GD**, Turner CH. Molecular-Level Solvation and Selectivity Behavior of Na^+, K^+, and Li^+ within Glycerol-Derived Solvents. *Chemical Engineering Science* **262**,117992. (DOI)

2022 **Barbosa GD,** Luz AM, Camargo CLM, Tavares FW, Turner CH. Molecular simulation of the structural and thermodynamic properties of n-alkane/brine interfacial systems with nonionic surfactants. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **655**, 130301. (DOI)

2022 Sermoud VM, **Barbosa GD**, Vernin NS, Barreto AG, Tavares FW. The impact of the adsorbent energy heterogeneities by multidimensional-multicomponent PC-SAFT-DFT. *Fluid Phase Equilibria* **562**, 113546. (DOI)

2022 Luz AM, Santos TJP, **Barbosa GD**, Camargo CLM, Tavares FW. A molecular study on the behavior of polyethoxylated alkyl ethers surfactants in a water/n-alkane interface. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **651,** 129627. (DOI)

2022 **Barbosa GD**, Dach E, Liu X, Yip NY, Turner CH. Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents. *Desalination* **537**, 115863. (DOI)

2022 **Barbosa GD**, Bara JE, Turner CH. Molecular simulation of glycerol-derived triether podands for lithium ion solvation. *Physical Chemistry Chemical Physics* **24**, 9459–9466. (DOI)

2022 Sermoud VM, **Barbosa GD**, Soares EA, Oliveira LH, Pereira MV, Arroyo PA, Barreto AG, Tavares FW. PCP-SAFT Density Functional Theory as a much-improved approach to obtain confined fluid isotherm data applied to sub and supercritical conditions. *Chemical Engineering Science* **267**, 1168662. (DOI)

2022 **Barbosa GD**, Bara JE, Weinman ST, CH Turner. Molecular aspects of temperature swing solvent extraction for brine desalination using imidazole-based solvents. *Chemical Engineering Science* **247**, 1168662. (DOI)

2022 **Barbosa GD**, X Liu, KE O'Harra, JE Bara, CH Turner. Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields. *Journal of Ionic Liquids* **2**, 100020. (DOI)

2021 **Barbosa GD**, CH Turner. Martini Coarse-Grained Model for Poly (alkylimidazolium) Ionenes and Applications in Aromatic Compound Extraction. *Macromolecules* **55**, 26. (DOI)

2021 **Barbosa GD**, Bara JE, Weinman ST, CH Turner. High-salinity brine desalination with amine-based temperature swing solvent extraction: a molecular dynamics study. *Journal of Molecular Liquids* **341**, 117359. (DOI)

2021 Sermoud VM, **Barbosa GD**, Soares EA, Barreto AG, Tavares FW. Exploring the multiple solutions of the classical density functional theory using metadynamics based method. *Adsorption*, 13th Brazilian Meeting on Adsorption.(DOI)

2021 Sappidi P, **Barbosa GD**, Rabideau B, Weinman S, Turner CH. Molecular simulation of high salinity brines in contact with diisopropylamine and tripropylamine solvents. *Industrial & Engineering Chemistry Research* **60**, 7925. (DOI)

2021 **Barbosa GD**, Camargo CLM, Freitas GB, Duncke ACP, Balestrin LBS, Poltronieri OCC, Nele M, Tavares FW. Molecular thermodynamics for aggregation of surfactants with alkylbenzene or

branched alkane tails: an experimental-modeling approach. *Fluid Phase Equilibria* **532**, 112918. (DOI)

2020 Sermoud VM, **Barbosa GD**, Barreto AG, Tavares FW. Quenched solid density functional theory coupled with PC-SAFT for the adsorption modeling on nanopores. *Fluid Phase Equilibria* **521**, 112700. (DOI)

2019 **Barbosa GD**, Travalloni L, Tavares FW, Castier M. Adsorption of gases on zeolitic imidazolate frameworks: modeling with equations of state for confined fluids and pore Size distribution estimation. *Industrial & Engineering Chemistry Research* 58, 19702. (DOI)

2019 Sermoud V, **Barbosa GD**, Barreto AG L, Tavares FW F. Reconstruction of the pore size distribution of porous materials: The influence of uncertainties in the gaseous adsorption experimental data. *Fluid Phase Equilibria* **494**, 93. (DOI)

2019 **Barbosa GD**, Travalloni L, Castier M, Tavares FW. Pore size distributions from extended Peng-Robinson equations of state for fluids confined in cylindrical and slit pores. *Fluid Phase Equilibria* **493**, 67. (DOI)

2018 **Barbosa GD**, Thibes R. A gauge invariant description for the general conic constrained particle from the FJBW iteration algorithm. *Brazilian Journal of Physics* **48**, 380. (DOI)

2018 **Barbosa GD**, Thibes R. A BRST formulation for the conic constrained particle. *Modern Physics Letters A* **33**, 1850055. (DOI)

2018 **Barbosa GD**, D'Lima ML, Daghash SMH, Castier M, Tavares FW, Travalloni L. Cubic equations of state extended to confined fluids: New mixing rules and extension to spherical pores. *Chemical Engineering Science* **184**, 52. (DOI)

2016 **Barbosa GD**, Castier M, Tavares FW, Travalloni L. Extending an equation of state to confined fluids with basis on molecular simulations. *Chemical Engineering Science* **153**, 212. (DOI)

2014 Thibes R, Batista E, **Barbosa GD**. Briefly revisiting the quantum mechanics supersymmetry algebra and group. *International Journal of Pure and Applied Mathematics* **97**, 99. (DOI)

2014 **Barbosa GD**, Ferreira RR, Thibes R. The classical particle coupled to external electromagnetic field symmetries and conserved quantities, *Revista Científica do Departamento de Química Exatas* **2**, 30. (PDF)

Conference Presentations

2022 **Barbosa GD**, Dach E, Liu X, Yip NY, Turner CH. "Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents". **Poster**, Foundations of Molecular Modeling and Simulation, Delavan, USA.

2022 Luz AM, Santos TJP, **Barbosa GD**, Camargo CLM, Tavares FW. A molecular study on the behavior of polyethoxylated alkyl ethers surfactants in a water/n-alkane interface. **Poster**, Foundations of Molecular Modeling and Simulation, Delavan, USA.

2021 **Barbosa GD**, Bara JE, Weinman ST, CH Turner. High-salinity brine desalination with amine-based temperature swing solvent extraction: a molecular dynamics study. **Oral**, AIChE meeting, Boston, USA.

2019 **Barbosa GD**, Camargo CLM, Freitas GB, Duncke ACP, Balestrin LBS, Poltronieri OCC, Nele M, Tavares FW. "Stability of Model Water-In-Oil Emulsions for Petroleum Systems". **Poster**, International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada.

2019 **Barbosa GD,** Sermoud V, Barreto AG L, Tavares FW F. "Thermodynamics Stability of Phase Transition For Inhomogeneous Fluids by Density Functional". **Poster**, International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada.

2019 **Barbosa GD,** Travalloni L, Castier M, Tavares FW. "Thermodynamic Modeling of Confined Fluids Via Extended Cubic Equations of State". **Poster**, International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada.

2017 Almeida MA, **Barbosa GD**, Travalloni L, Tavares FW. "Extension of an equation of state based on molecular simulation to the modeling of confined fluids.", Brazilian Congress of Applied Thermodynamics (CBTermo), Porto Alegre, RS.

2016 **Barbosa GD**, Travalloni L, Tavares FW. "Modeling of confined fluids via molecular simulation and equation of state". **Oral**, International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal.

2013 **Barbosa GD**, Batista E, Thibes R. "Briefly revisiting the supersymmetry algebra and group of one dimensional quantum mechanics". **Oral**, XXXI Physics Congress of the north and northeast of Brazil (XXXIEFNN), Campina Grande, Brazil.

2012 **Barbosa GD**, Ferreira RR, Thibes R. "On the quantization of particle on a circle as a constrained system". **Poster**, IV Latin American Congress of Mathematicians (CLM-UMALCA), Cordoba, Argentina.

2011 **Barbosa GD**, Oliveira MP, Thibes R. "Applications of group theory in molecular symmetry". **Poster**, XXIX Physics Congress of the north and northeast of Brazil (XXXI-EFNN), Mossoro, Brazil

2011 **Barbosa GD**, Ferreira RR, Thibes R. "The classical particle coupled to external electromagnetic field symmetries and conserved quantities". **Poster**, National Congress of Physicists, Foz do Iguaçu, Brazil.

2010 **Barbosa GD**, Thibes R. "Lagrange multipliers in analytical mechanics - determining forces based on geometric constraints". **Poster**, Biennial of the Brazilian Mathematical Society (BSBM), João Pessoa, Brazil.

University Service

Federal University of Rio de Janeiro. Participation on evaluation committees of undergraduate projects

2016 Rocha MM, "Study of the use of concentrated solar energy in distillation tower".

State University of Southwestern Bahia. Teaching assistant

2013 Linear Algebra.
2012 Quantum Mechanics.
2011 Differential and Integral Calculus.
2011 Differential and Integral Calculus II.
2010 Differential and Integral Calculus I.
2009 Physics I.
2009 General Chemistry I.

Other Skills

English: Proficient
Spanish: Proficient
Portuguese: Fluent

Graduate Coursework

- Process Engineering (UFRJ)
- Applied Thermodynamic (UFRJ)
- Statistical Mechanics (UFRJ)
- Numerical Methods in Chemical Engineering (UFRJ)
- Transport Phenomena (UFRJ)
- Mathematical Methods in Chemical Engineering (UFRJ)
- Experimental Statistics (UFRJ)
- Bioreactor and Biosystems (UFRJ)
- Statistical Thermodynamics and Molecular Simulation (UFRJ)
- Functional Analysis (UFRJ)
- Structure and Properties of Colloidal Dispersions - Water and Oil Emulsions (UFRJ)
- Interfacial Phenomena (UFRJ)
- Non-Equilibrium Thermodynamics (UFRJ)