Henrique Musseli Cezar

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Ph.D in Physics, works with computational physics/chemistry and developing scientific software. My research interests are in the development of new methods for molecular simulation and the use of molecular simulation and quantum mechanics calculations to solve problems in physical chemistry, biochemistry and materials science.

Education and positions

2020– **Postdoctoral researcher, Institute of Physics, University of São Paulo**
Computational nanofluidics studies on the confinement effects on fluid-solid interfaces.
FAPESP Fellowship - Supervisor: Dr. Caetano R. Miranda

2018–2019 **Postdoctoral researcher, Institute of Physics, University of São Paulo**
Development and applications of Configurational Bias Monte Carlo Method in dyes of interest to organic solar cells
CAPES Fellowship - Supervisor: Dr. Kaline R. Coutinho

2015–2018 **Ph.D. in Physics, Institute of Physics, University of São Paulo**
Implementation and Development of Efficient Algorithm for Intramolecular Deformation with the Monte Carlo Method
CNPq Ph.D. Fellowship - Advisor: Dr. Kaline R. Coutinho

2013–2015 **Master's in Computational Physics, São Carlos Institute of Physics, University of São Paulo**
Implementation of the Parallel Tempering Monte Carlo Method to the Study of Thermodynamic Properties of Nanoclusters
FAPESP Master Fellowship - Advisor: Dr. Juarez L. F. Da Silva

2009–2012 **B.S. in Computational Physics, São Carlos Institute of Physics, University of São Paulo**
Undergraduate research entitled: Fluid Dynamics in Porous Media with Lattice Boltzmann
CNPq Scientific Initiation Fellowship - Advisor: Dr. Leonardo P. Maia

Complementary Education

2018 **Short Course:** I GPU Computing Workshop (Duration: 11h). University of São Paulo.
2016 **Short Course:** 4th Workshop HPC - USP/Rice (Duration: 8h). University of São Paulo.
2015 **Coursera Online Course:** Algorithms: Design and Analysis, Part 1. (Duration: 36h). Stanford University.
2006–2008 **Technical Course:** Informatics. Colégio Divino Salvador.

Awards

2020 **Top Downloaded Paper**: "Solvent effect on the syn/anti conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods", Wiley.
2019 **3rd place** in the best flash talks award at the XX Simpósio Brasileiro de Química Teórica.
2017 **Best poster** award at the XIX Simpósio Brasileiro de Química Teórica.
2017 **Among the 12 finalists** of the "My Thesis in 180 Seconds", organized by Swissnex Brazil.
2015 **Honorable mention** at the best poster award of the II Workshop on Biomolecular Theory-Experiment Inter-

play.

Teaching Experience

2019 **Física II**: Teacher for the second semester physics class at the Escola Politécnica of the University of São Paulo.
2019 **Física I**: Teacher for the first semester physics class at the Escola Politécnica of the University of São Paulo.
2017 **Física Moderna I**: Teaching assistant for the introductory modern physics class of the Physics course of University of São Paulo, under the supervision of Prof. Dr. Sylvio Canuto.

Research overview

My research is mainly focused on the development of algorithms for classical molecular simulation. Specifically, I have experience implementing and using Monte Carlo methods and using molecular dynamics for the simuation of solute-solvent and interface systems. During my Master I have implemented a parallel tempering Monte Carlo algorithm with several options in GOTNano, and have used this same software, together with FHI-aims, to investigate the properties of nanoclusters. In my PhD I developed a Configurational Bias Monte Carlo method for the efficient simulation of flexible molecules in solution, showing that the method may perform better than standard molecular dynamics for the sampling of systems with high energy barriers between conformers.
Even though most of my research has been in developing and implementing computational methods, I also have interest in combining different techniques to solve problems in physical chemistry and materials science. In my career I have used different methods such as molecular dynamics for the simulation of molecular systems, global optimization algorithms to search for the putative global minimum configurations, clustering algorithms to analyze data from simulation, fitting of interatomic potentials and density functional theory to investigate the electronic structure and absorption spectra of molecules and transition metal nanoclusters. All these methods form a useful toolset that can be used to investigate matter in the solid, liquid and gas phases, as well as its interfaces.
In my most recent project, I have been using Grand Canonical Monte Carlo and molecular dynamics to investigate confinement effects on gas-solid and fluid-solid interfaces. Some of my efforts have been in validating and fitting interatomic potentials for these simulations.

Computational Skills

I am proficient with the programming languages (from more to less proficient): Fortran (legacy and modern), Python, C, Bash and C++. I have experience with OpenMP parallelization, code profiling and optimization. I also have some knowledge in message passaging parallelization with MPI and GPU and shared memory parallelization with OpenACC, even though I haven't used those in a production environment. I know how to use the Git and SVN version control systems.
Concerning scientific software, I am familiar with DICE, GOTNano, Cassandra, GROMACS and LAMMPS for molecular simulation. For electronic structure calculations I have used Gaussian, FHI-AIMS and Quantum Espresso.

Software development

Apart from several scripts and smaller software, my major contributions are developing:

Cezar HM, Canuto S, Coutinho K
DICE
https://portal.if.usp.br/dice
A Monte Carlo code for the molecular simulation of liquids and gases using classical force fields. My main contribution is the coding and development of a Configurational Bias Monte Carlo method used to sample the internal degrees of freedom of the molecules. I have also implemented shared memory parallelization and improved the overall performance. The code is written in Fortran and has OpenMP parallelization.

Rondina GG, **Cezar HM**, Da Silva JLF

GOTNano

A code for global optimization and sampling of thermodynamic properties of nanoclusters. My main contribution is the implementation of the Parallel Tempering Monte Carlo algorithm used to sample the thermodynamic properties. The code is written in C and has OpenMP parallelization.

Cezar HM

Clustering Trajectory

https://github.com/hmcezar/clustering-traj

A parallel Python script that performs clustering over an atomistic molecular simulation trajectory, searching for the minimum RMSD between each structure and classifying using one of the many clustering algorithms available in the machine learning library sklearn.

Cezar HM

DICEtools

https://github.com/hmcezar/dicetools

A package containing several scripts used to prepare DICE inputs and analyze simulation data.

Cezar HM

pdb2lmp

https://github.com/Sampa-USP/pdb2lmp

Create LAMMPS topologies from structure files.

Cezar HM

nanotube-tools

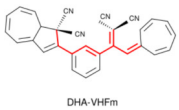
https://github.com/Sampa-USP/nanotube-tools

Set of tools to manipulate, create and characterize nanotubes.

Publications

h-index: 5, citations: 69 (September 12th, 2021)
Publons, Google Scholar

Published



Cardenuto MH, **Cezar HM**, Mikkelsen KV, Sauer SPA, Coutinho K, Canuto S

A QM/MM study of the conformation stability and electronic structure of the photochromic switches derivatives of DHA/VHF in acetonitrile solution

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 251:119434, 2021 · DOI

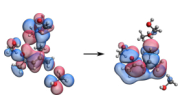
The absorption spectra of photoswichtes composed of two units of photochromic molecules, namely, dihydroazulene (DHA)/vinylheptafulvene(VHF) is studied including explicit solvation and considering the rotamers that are exhibited at room temperature. We obtain the free energies and perform clustering analysis, rationalizing the absorption spectra at the different solvents.

Cezar HM, Canuto S, Coutinho K

DICE: A Monte Carlo code for molecular simulation including Configuration Bias Monte Carlo method

Journal of Chemical Information and Modeling 60:3472, 2020 · DOI

We describe DICE, a software that uses Monte Carlo methods to perform molecular simulation, focusing on solute-solvent systems. We introduce our implementation of the Configurational Bias Monte Carlo method that includes new methodological developments and employ the method to study different molecules such as alkanes, 1,2-dichloroethane and a large boron phtalocyanine.

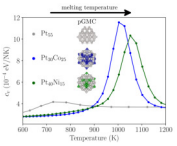


Cezar HM, Canuto S, Coutinho K

Understanding the Absorption Spectrum of Mesityl Oxide Dye in Solvents of Different Polarities

Journal of Molecular Liquids 307:112924, 2020 · DOI

We investigate the conformational and solvent effects on the UV/vis spectroscopy of the mesityl oxide dye. We show that a correct description of the syn/anti population and the use of explicit solvent molecules is fundamental to describe the solvatochromic shifts.



Cezar HM, Rondina GG, Da Silva JLF

Thermodynamic Properties of 55-Atom Pt-based Nanoalloys: Phase Changes and Structural Effects on the Electronic Properties

Journal of Chemical Physics 151:204301, 2019 · DOI

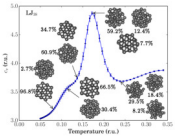
We investigate the effects of temperature on the structure of Pt-based nanoalloys, performing Parallel Tempering Monte Carlo simulations using many-body potentials and DFT calculations to see how the structural changes affect the density of states. We show that the melting temperature of the Pt nanocluster is increased by alloying it with Co and Ni, and that the temperature effects on the structures shift the d-band center towards the HOMO, indicating a greater catalytic activity.

Cezar HM, Canuto S, Coutinho K

Solvent effect on the syn/anti conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods

International Journal of Quantum Chemistry 119:e25688, 2019 · DOI

We compare the Configurational Bias Monte Carlo (CBMC) and molecular dynamics (MD) sampling of the mesityloxide molecule in gas phase and solution, showing that that while CBMC performs an ergodic sampling, MD has troubles overcoming the 10 kcal/mol energy barrier between the syn and anti conformations.

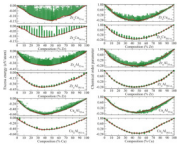


Cezar HM, Rondina GG, Da Silva JLF

Parallel Tempering Monte Carlo Combined with Clustering Euclidean Metrics Analysis to Study the Thermodynamic Stability of Lennard-Jones Nanoclusters

Journal of Chemical Physics 146:064114, 2017 · DOI

We use a clustering algorithm to analyze trajectories from Parallel Tempering Monte Carlo simulations of Lennard-Jones nanoclusters, identifying the phase changes and most most frequent structures with great accuracy using a very simple approach.



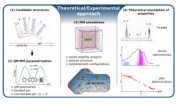
De Souza DG, **Cezar HM**, Rondina GG, De Oliveira MF, Da Silva JLF

A Basin-hopping Monte Carlo Investigation of the Structural and Energetic Properties of 55- and 561-atom Bimetallic Nanoclusters: the Examples of the ZrCu, ZrAl, and CuAl Systems

Journal of Physics: Condensed Matter 28:175302, 2016 · DOI

We report a basin-hopping Monte Carlo investigation of the structural and energetic properties of bimetallic ZrCu, ZrAl, and CuAl nanoclusters with 55 and 561 atoms, showing how the atoms of the different species are distributed in the structure, and a trend of more spherical structures at 50-50 compositions.

Under review



Franco LR, Toledo KCF, Matias TA, Benavides PA, **Cezar HM**, Araujo CMG, Coutinho K, Araki K

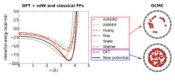
Unraveling the acid-base characterization and solvent effects on structural and electronic properties of a bis-bidentated bridging ligand

Physical Chemistry Chemical Physics ·

We report a combined theoretical-experimental study of the bis(2-pyridyl)-bis-imidazole in solution, determining the protonation sites, most favorable conformations and absorption spectra in different solvents.

In preparation

I have five manuscripts in different steps of preparation, of which I highlight the three manuscripts below that are under the review of the coauthors and should be submitted in the next weeks.



Cezar HM, Lanna TD, Damasceno DA, Kirch A, Miranda CR

Revisiting greenhouse gases adsorption in carbon nanostructures: advances through a combined first-principles and molecular simulation approach

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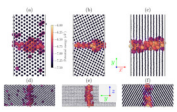
We investigate the adsorption properties of CH_4 and CO_2 in carbon nanotubes (CNTs) using different force fields within the Lorentz-Berthelot combining rules. Using density functional theory we found that the adsorption energies are underestimated for all the force fields. We fitted new cross Lennard-Jones parameters and investigated the effects of the different parametrization in the adsorption properties using Grand Canonical Monte Carlo.



Salvador CAF, **Cezar HM**, Miranda CR

Atomistic simulations of symmetric tilt grain boundaries in Nb-1Zr alloys

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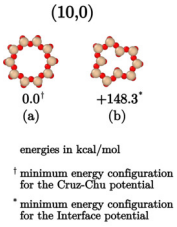
We investigate the mechanical properties of three different symmetric tilt grain boundaries (STBs) at the Nb – 1 Zr at.% compositions. Using non equilibrium molecular dynamics simulations and Monte Carlo moves, we obtain that the Zr stays at the grain boundray, and the addition of small amounts of Zr can help pin the STBs. We also analyze the stress-strain curves and fracture patterns.



Cezar HM, Miranda CR

Water adsorption in ultrathin silica nanotubes

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We investigate the structure and adsorption properties for three sizes of SiO_2 nanotubes. We consider some of the most used force fields for describing silica and compare the nanotube structures with density functional theory and water adsorption properties by comparison with experimental silicalite results. Finally, we report water adsorption isotherms for the nanotubes and rationalize the confinement effects looking at the accessible volume of each nanotube.

Invited and contributed talks

São Carlos, SP
Sep 2019

DICEtools and Clustering-Traj: From simulation setup to data analysis
III New Energies Innovation Center - Computational Material Science Division Workshop

São Carlos, SP
Feb 2019

Monte Carlo Methods
II New Energies Innovation Center - Computational Material Science Division Workshop (Invited talk)

Brasília, DF
Sep 2018

Comparison Between Configurational Bias Monte Carlo and Molecular Dynamics Sampling for Sampling Conformational Stability with High Energy Barriers
VII SeedMol

Livorno, Italy
Aug 2017

Configurational Bias Monte Carlo of Molecules in Solvent and Comparison with Molecular Dynamics
Coding Solvation Workshop

Recife, PE
May 2017

Comparsion of the sampling of Molecular Dynamics and Configurational Bias Monte Carlo for 1,2- dichloroethane and octane.
III Advanced School on Biomolecular Simulation

Rio de Janeiro, RJ
Mar 2017

How Indiana Jones is actually a bad explorer when it comes to molecules and how I can do better
Finals of My Thesis in 180 seconds (Swissnex Brazil)

João Pessoa, PB
Sep 2014

Parallel Tempering Monte Carlo Investigation of Phase-Changes in Nanoclusters
XIII Encontro da SBPMat

Poster presentation

Online
Feb 2021

Revisiting greenhouse gases adsorption in carbon nanotubes: advances by ab initio optimized potentials
20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

João Pessoa, PB
Nov 2019

Conformational effects on the solvatochromism of mesityl oxide: the importance of an ergodic sampling
XX SBQT

São Carlos, SP
Feb 2019

Application of Configurational Bias Monte Carlo method for the simulation of dyes and porous nanoparticles
II New Energies Innovation Center - Computational Material Science Division Workshop

São Carlos, SP
Oct 2018

Implementation of Configurational Bias Monte Carlo method for the simulation of flexible molecules in solution
I New Energies Innovation Center - Computational Material Science Division Workshop

Águas de Lindóia, SP
Nov 2017

Implementation of Configurational Bias Monte Carlo Method to Sample Flexible Solute in Solvent Media
XIX SBQT

Munich, Germany
Aug 2017

Configurational Bias Monte Carlo method to sample molecular flexibility: The case of octane and 1,2-dichloroethane
WATOC 2017

Maresias, SP
Aug 2015

Parallel Tempering Monte Carlo applied to the study of transition-metal nanoclusters
II Workshop on Biomolecular Theory-Experiment Interplay

Trieste, Italy
Aug 2013

Thermodynamic properties of nanoclusters: An investigation with Parallel Tempering Monte Carlo
Density Functional Theory and Beyond: Computational Materials Science for Real Materials

São Paulo, SP
Oct 2012

Estudo de dinâmica de fluidos em meios porosos com métodos de Boltzmann na rede
XX SIICUSP

Conferences organized

Recife, PE
May 2017

III Advanced School on Biomolecular Simulation
Member of the local committee.