

Henrique Musseli Cezar



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Ph.D in Physics, working 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

- 2022- **Postdoctoral researcher, Hylleraas Centre for Quantum Molecular Sciences, University of Oslo**
Further developments in the Hamiltonian hybrid particle-field molecular dynamics and use with metainference
Supervisor: Prof. Michele Casella
- 2020-2022 **Postdoctoral researcher, Institute of Physics, University of São Paulo**
Computational nanofluidics studies on the confinement effects on fluid-solid interfaces.
FAPESP Fellowship - Supervisor: Prof. 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: Prof. 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: Prof. 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: Prof. 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: Prof. Leonardo P. Maia

Approved grants

- 2020 FAPESP Two-years Postdoc Fellowship.
2013 FAPESP Two-years Masters Fellowship.

Awards

- 2022 **Best PhD thesis** in the field of atomic and molecular physics, by the Brazilian Physical Society.
2022 **Honorable mention** at the annual prize of the Institute of Physics, University of São Paulo, at the "Highlight in instrumentation and software development" category.
- 2020 **Top Downloaded Paper:** "Solvent effect on the syn/anti conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods", Wiley.

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| 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 Interplay. |

Teaching Experience

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| 2019 | Física II (Basic Physics II): Teacher for the second semester physics class for the mechanical engineering majors at the Escola Politécnica – University of São Paulo. |
| 2019 | Física I (Basic Physics I): Teacher for the first semester physics class for the mechanical engineering majors at the Escola Politécnica – University of São Paulo. |
| 2017 | Física Moderna I (Modern Physics I): Teaching assistant for the introductory modern physics class for the physics majors of the Institute of Physics – University of São Paulo, under the supervision of Prof. Dr. Sylvio Canuto. |

Research Experience

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 molecular dynamics for the simulation of solute-solvent, interface and biomolecular systems. During my Master I have implemented a parallel tempering Monte Carlo algorithm in GOTNano, and have used this same software, together with FHI-aims, to investigate the properties of transition metal nanoclusters. In my PhD I developed a Configurational Bias Monte Carlo method for the efficient simulation of flexible molecules in solution, and implemented it in DICE, showing that the method may perform better than standard molecular dynamics for the sampling of systems with high energy barriers between conformers. More recently, I have been maintaining Hylleraas MD, a Hamiltonian hybrid particle-field software, in which I have implemented a interface with PLUMED. I have also given contributions to PLUMED development regarding the implementation of small angle neutron scattering (SANS) and the Python MPI interface. In my career I have used 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 simulations, fitting of interatomic potentials, and density functional theory to investigate the electronic structure and absorption spectra of molecules and transition metal nanoclusters.

Recently, I have been employing metainference, a Bayesian inference method, to bias coarse-grain simulations towards agreement with small angle scattering spectra in collaboration with experimentalists.

I'm also leading a project to develop a method for the classification of structures in solute-solvent systems. Together with a PhD student from the University of São Paulo, we are developing a software package called ClustTraj.

Languages

Portuguese (native), English (fluent) and Norwegian (novice).

Technical Skills

I am proficient with Python, Fortran, C, Bash, and C++, and have experience with OpenMP and MPI parallelization, code profiling, and optimization. I also have some experience using GitHub actions for automating unit testing, deploying documentation, and publishing Python packages.

Concerning scientific software, I am familiar with DICE, GOTNano, HylleraasMD, Cassandra, GROMACS, and LAMMPS for molecular simulations. For electronic structure calculations, I have some experience with Gaussian, FHI-AIMS and Quantum Espresso.

Software development

[GitHub](#), [GitLab](#)

Apart from many 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, and parallelization. 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.

Ledum M, Carrer M, Sen S, Li X, Cezar HM, Casella M, Bore SL

Hylleraas MD

<https://github.com/Casella-Group-Uo/HyMD>

A molecular dynamics software that implements the Hamiltonian hybrid particle-field method. I am currently the main maintainer of the software, and my main contribution is the PLUMED interface. HyMD is written in Python and Fortran.

Cezar HM, Ribeiro RB

ClustTraj

<https://github.com/hmcezar/clusttraj>

A parallel Python package that performs clustering over an atomistic molecular simulation trajectory, searching for the minimum RMSD between each structure and classifying using hierarchical clustering, with options to deal with solute solvent systems.

Cezar HM

DICEtools

<https://github.com/hmcezar/dicetools>

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

Publications

h-index: 8, citations: 149 (October 4th, 2023)

[Web of Science](#), [Scopus](#), [ORCID](#), [Google Scholar](#)

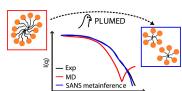
Published

Cezar HM, Casella M

SANS Spectra with PLUMED: Implementation and Application to Metainference

Journal of Chemical Information and Modeling 63:4979, 2023 · [DOI](#)

In this Application Note we describe our implementation of Small Angle Neutron Scattering spectra including the use of a resolution function and its application to metainference simulations.

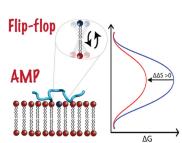


Carrer M, Nielsen JE, Cezar HM, Lund R, Casella M, Soares TA

Accelerating Lipid Flip-Flop at Low Concentrations: A General Mechanism for Membrane Binding Peptides

The Journal of Physical Chemistry Letters 14:7014, 2023 · [DOI](#)

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.

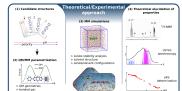


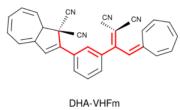
Franco LR, Toledo KCF, Matias TA, Benavides PA, Cezar HM, Araujo CMG, Coutinho K, Araki K

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

Physical Chemistry Chemical Physics 24:10222, 2022 · [DOI](#)

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.





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 photoswitches 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.

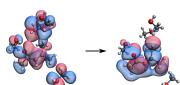


Cezar HM, Canuto S, Coutinho K

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 phthalocyanine.

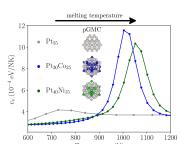


Cezar HM, Canuto S, Coutinho K

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.

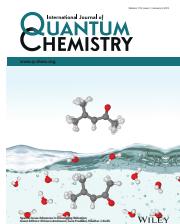


Cezar HM, Rondina GG, Da Silva JLF

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.

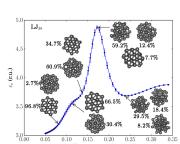


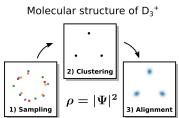
Cezar HM, Canuto S, Coutinho K

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 while CBMC performs an ergodic sampling, MD has troubles overcoming the 10 kcal/mol energy barrier between the syn and anti conformations.

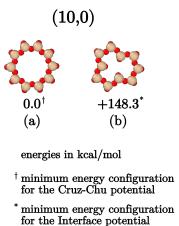




Lang L, Cezar HM, Adamowicz L, Pedersen TB
Finding Molecular Structure in Molecular Wavefunctions

ChemRxiv · [DOI](#)

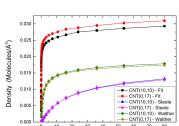
In this manuscript we use Monte Carlo to sample an all-particle wavefunction, and propose a new definition of molecular structure beyond the Born-Oppenheimer approximation.



Cezar HM, Miranda CR
Water adsorption in ultrathin silica nanotubes

arXiv · [DOI](#)

We investigate the structure and adsorption properties for three sizes of SiO_2 nanotubes, understanding the adsorption in terms of the accessible volume.

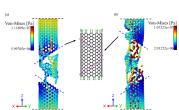


Martins Junior CA, Cezar HM, Damasceno DA, Miranda CR

Effects of van der Waals interaction on the N2 adsorption on carbon nanotubes: proposal of new force field parameters

arXiv · [DOI](#)

We investigate the adsorption of N_2 in CNTs, proposing an interatomic potential that correctly describe the energies for different adsorption sites, leading to a more accurate description of adsorption isotherms.



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

Mechanical and adsorption properties of greenhouse gases filled carbon nanotubes

arXiv · [DOI](#)

Using molecular simulations we investigate the mechanical stability of CNTs filled with mixtures of CO_2 and CH_4 , finding that under compression several parameters can play a role in the in the materials response.

Selected 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

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 Brazilian Materials Research Society Meeting

Conferences organized

Recife, PE
 May 2017

III Advanced School on Biomolecular Simulation

Member of the local committee.