

# Henrique Musseli Cezar



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post Hylleraas Centre for Quantum Molecular Sciences and Department of Chemistry, Room V208, University of Oslo, PO Box 1033 Blindern, 0315 Oslo, Norway

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-	<b>Postdoctoral researcher, Hylleraas Centre for Quantum Molecular Sciences, University of Oslo</b> Further developments in the Hamiltonian hybrid particle-field molecular dynamics and use with metainference Supervisor: Prof. Michele Casella
2020–2022	<b>Postdoctoral researcher, Institute of Physics, University of São Paulo</b> Computational nanofluidics studies on the confinement effects on fluid-solid interfaces. FAPESP Fellowship - Supervisor: Prof. Caetano R. Miranda
2018–2019	<b>Postdoctoral researcher, Institute of Physics, University of São Paulo</b> 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	<b>Ph.D. in Physics, Institute of Physics, University of São Paulo</b> 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	<b>Master's in Computational Physics, São Carlos Institute of Physics, University of São Paulo</b> 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>B.S. in Computational Physics, São Carlos Institute of Physics, University of São Paulo</b> 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	<b>Best PhD thesis</b> in the field of atomic and molecular physics, by the Brazilian Physical Society.
2022	<b>Honorable mention</b> at the annual prize of the Institute of Physics, University of São Paulo, at the "Highlight in instrumentation and software development" category.
2020	<b>Top Downloaded Paper:</b> "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 Interplay.

## Teaching Experience

2019	<b>Física II (Basic Physics II):</b> Teacher for the second semester physics class for the mechanical engineering majors at the Escola Politécnica – University of São Paulo.
2019	<b>Física I (Basic Physics I):</b> Teacher for the first semester physics class for the mechanical engineering majors at the Escola Politécnica – University of São Paulo.
2017	<b>Física Moderna I (Modern Physics I):</b> 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.

Even though most of my research has been in developing and implementing computational methods, I also have an interest in combining different techniques to solve problems in physical chemistry and materials science. 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. Combined, these methods provide a set of tools that can be used to investigate matter in the solid, liquid, and gas phases, as well as its interfaces.

In my recent projects, besides method development, 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. As one of the results, a Python package called ClustTraj is being developed. The project is being carried with a Brazilian PhD student from the University of São Paulo.

## Computational Skills

I am proficient with Python, Fortran, C, Bash, and C++. I have experience with OpenMP and MPI parallelization, code profiling, and optimization. GitHub is where I host most of my projects, and most are open source. I have some experience using GitHub actions for unit tests, deploying documentation, and 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. 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.

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.

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>

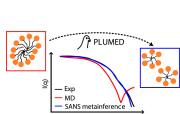
A package containing several scripts used to prepare DICE inputs and analyze simulation data.

## Publications

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

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

### Published

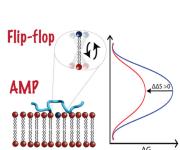


Cezar HM, Casella M

#### **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.

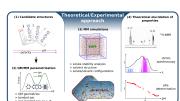


Carrer M, Nielsen JE, Cezar HM, Lund R, Casella M, Soares TA

#### **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.

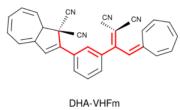


Franco LR, Toledo KCF, Matias TA, Benavides PA, Cezar HM, Araujo CMG, Coutinho K, Araki K

#### **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.

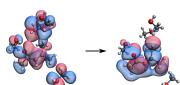


Cezar HM, Canuto S, Coutinho K

## 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.

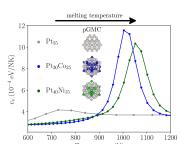


Cezar HM, Canuto S, Coutinho K

## 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.

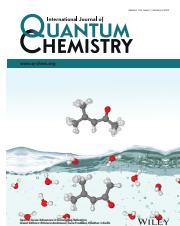


Cezar HM, Rondina GG, Da Silva JLF

## 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.

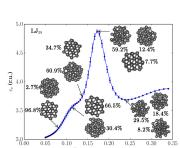


Cezar HM, Canuto S, Coutinho K

## 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.

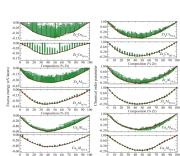


Cezar HM, Rondina GG, Da Silva JLF

## 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 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.

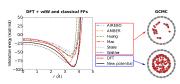
## Preprints and submitted manuscripts

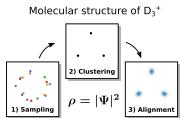
Cezar HM, Lanna TD, Damasceno DA, Kirch A, Miranda CR

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

arXiv · DOI

We investigate the adsorption properties of CH<sub>4</sub> and CO<sub>2</sub> in carbon nanotubes (CNTs) using different force fields, showing that the adsorption energies are underestimated. A new interatomic potential is proposed based on the first-principles calculations.



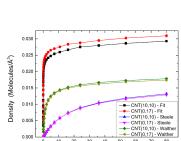
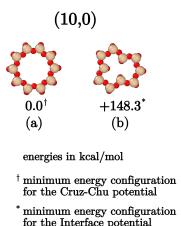


Lang L, Cezar HM, Adamowicz L, Pedersen TB

## 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.

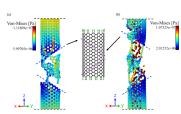


Martins Junior CA, Cezar HM, Damasceno DA, Miranda CR

## 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.

## 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 Brazilian Materials Research Society Meeting

## Conferences organized

Recife, PE  
May 2017

### **III Advanced School on Biomolecular Simulation**

Member of the local committee.