Henrique Musseli Cezar

email	h.m.cezar@kjemi.uio.no
github	https://github.com/hmcezar
orcid	0000-0002-7553-0482
linkedin	https://www.linkedin.com/in/hmcezar
mobile	+47 968 17 973
post	Hylleraas Centre for Quantum Molecular Sciences and Department of Chemistry, 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 such methods 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 Cascella

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 Institue 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.

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 **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, interfacial and biomolecular systems. At the Hylleraas Centre, 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. On top of the molecular simulation methods, I have some experience with global optimization algorithms, clustering algorithms, fitting of interatomic potentials, and density functional theory.
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. With my collaborators, we are exploring the use of machine learning potentials (NequIP and Allegro) and their integration with the the Hylleraas Software Platform. I'm also leading a project to develop a method for the classification of structures in solute-solvent systems (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. My Python projects have used libraries like NumPy, Pandas, SciPy, mpi4py, scikit-learn and matplotlib. I also have some experience using GitHub actions for automating unit testing, deploying documentation, and publishing Python packages. I know how to use HPC systems like SLURM and PBS, and have experience with Docker and Singularity containers.
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 (see the links above), 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**, Cascella M, Bore SL

Hylleraas MD

https://github.com/Cascella-Group-UiO/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 and uses MPI for parallelization.

Cezar HM, Ribeiro RB

ClustTraj

https://github.com/hmcezar/clusttraj

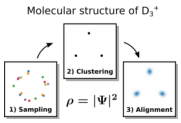
A parallel Python package that performs clustering over an atomistic molecular simulation trajectory, searching for the minimum RMSD between each structure and classifying using hierarchical clustering, with options to deal with solute solvent systems.

Publications

h-index: 8, citations: 162 (May 24th, 2024)

Web of Science, Scopus, ORCID, Google Scholar

Published

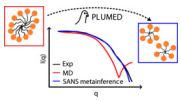


Lang L, **Cezar HM**, Adamowicz L, Pedersen TB

Quantum Definition of Molecular Structure

Journal of the American Chemical Society 146:1760, 2024 · 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.

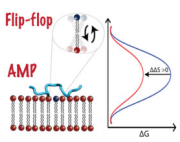


Cezar HM, Cascella M

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.

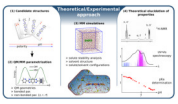


Carrer M, Nielsen JE, **Cezar HM**, Lund R, Cascella M, Soares TA

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 show that the flip-flop of lipids in a membrane can be accelerated by the presence of peptides. The mechanism is entropic, due to the restriction in mobility of lipids introduced by the presence of the peptide, and is not necessarily driven by smaller enthalpic barriers.

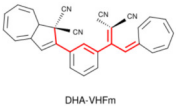


Franco LR, Toledo KCF, Matias TA, Benavides PA, **Cezar HM**, Araujo CMG, Coutinho K, Araki K

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

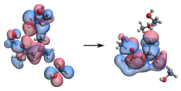
The absorption spectra of photoswichtes composed of two units of photochromic molecules, namely, dihydroazulene (DHA)/vinylheptafulvene(VHF) is studied including explicit solvation and considering the rotamers that are exhibited at room temperature. We obtain the free energies and perform clustering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

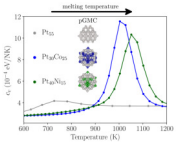


Cezar HM, Canuto S, Coutinho K

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.

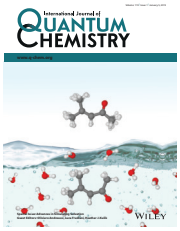


Cezar HM, Rondina GG, Da Silva JLF

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.

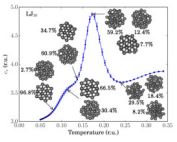


Cezar HM, Canuto S, Coutinho K

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.

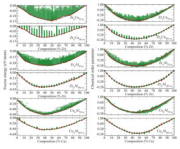


Cezar HM, Rondina GG, Da Silva JLF

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.



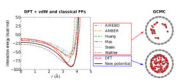
De Souza DG, **Cezar HM**, Rondina GG, De Oliveira MF, Da Silva JLF

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.

Preprints and submitted manuscripts

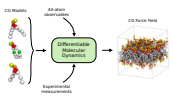


Cezar HM, Lanna TD, Damasceno DA, Kirch A, Miranda CR

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_4 and CO_2 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.

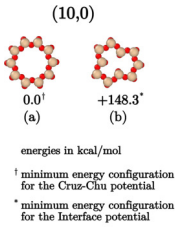


Carrer M, **Cezar HM**, Bore SL, Ledum M, Cascella M

Learning Force Field Parameters from Differentiable Particle-Field Molecular Dynamics

ChemRxiv · DOI

We develop a differentiable molecular dynamics software based on the Hamiltonian hybrid particle-field formalism, and use it to establish a protocol for automated optimization of force field parameters.

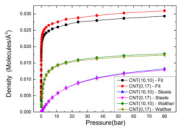


Cezar HM, Miranda CR

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.

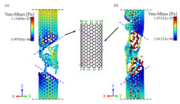


Martins Junior CA, **Cezar HM**, Damasceno DA, Miranda CR

Effects of van der Waals interaction on the N_2 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.