# CURRICULUM VITÆ

# ÁLVARO DE JESÚS OCHOA CALLE

## MY INTEREST

I have been waiting for an opportunity to advance my knowledge of science, and I believe that working with you is the opportunity that I have been waiting for. I acknowledge that achieving a postdoctoral position, particularly in a prestigious university, is not easy. However, I am persistent and optimistic that my background and skillset will distinguish me.

One of the most important contributions I have made, arose during my PhD studies, which was finding a better theoretical description for the systems under pressure, particularly, for the $\epsilon$ phases of the solid oxygen. The phase transition from diamagnetic $\epsilon$ to superconducting $\zeta$ phase at 96 GPa was also studied.

I find particularly interesting the theoretical description of systems under extreme conditions. The mathematical tools in conjunction with computational software can be used to help understand the exotic properties that these systems pose. My interests lie in the use of mathematical tools, i.e. stochastic or deterministic methods, to describe these phenomenon.

Of the two postdoctoral positions, I find The Physics at Extreme Conditions most interesting. Nevertheless, The planetary work also interests me because it is a new field of research.

## PERSONAL INFORMATION


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| *Date of birth* | October 21, 1987 |
| *Place of birth* | Venecia, Antioquia- Colombia |
| *Gender* | Male |
| *Citizenship* | Colombian |
| *Marital status* | Single |
| *Address* | Calle Sur 23 Mz 25; Lt 220; Colonia Leyes de Reforma; CP 09310, Delegación: Iztapalapa; Ciudad de México-México. |
| *email* | ajochoacalle@gmail.com |
| *Cell phone* | +52 55 35 01 96 36 |

## PRESENT POSITION

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| *From july 2017 to july 2018* | Postdoctoral position<br>Metropolitan Autonomous University<br>Ciudad de México-México |

## FORMER POSITION

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| *2015-2017* | Associate professor<br>EAFIT University<br>Medellín-Colombia |
| *2009–2010* | Youngh research of the condensed matter group<br>University of Antioquia<br>Medellín-Colombia |

## EDUCATIONAL BACKGROUND

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| *Jun 17, 2015* | PhD in physics *with honorific mention*<br>Autonomous University of the Morelos State<br>Cuernavaca-México |
| *July, 2011* | Degree in Physics<br>University of Antioquia<br>Medellín-Colombia |
| *December, 2004* | High School<br>Educational Institution San José of Venecia<br>Venecia, Antioquia-Colombia |

## LANGUAGES

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| *English* | Good command |
| *Spanish* | First language |

## SKILLS

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| *Fortran, C++ and Mathematica*<br>*Languages programming* | I am experienced in the use of these language |

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| *Crystal code* | Crystal is a program for cristalline systems and used localized atomic basis set. For systems under hidrostatic pressure, Crystal is a better programing tool for the best description to these periodic systems. I am highly trained in the use of this code. During my PhD, I studied the some subroutines related with phonon spectre (IR and Raman) |
| *VASP and Quantum espresso* | My knowledge is limited, however I am a fast learning |
| *Molpro and Gaussian packages* | I am experienced in the use of these languages |

## SHORT RESEARCH STAYS

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| *France 2012* | Paul Sabatier University<br>Quantum Monte Carlo method applied to the $\varepsilon$ phase of the solid oxygen-Cluster approximation<br>Dr. Michel Caffarel.<br>Toulouse-France |
| *Italy 2013* | University of Turin.<br>Converging of the enthalpy respect to the threshold of the bielectronic integrals using GGA and hybrid type functionals in the Crystal code<br>Dr. Roberto Dovesi.<br>Turin-Italy |

## PARTICIPATION IN CONFERENCES AND WORKSHOPS

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| *2012* | Talk. XI Mexican meeting of theoretical physical chemistry. November 8-10 Toluca de Lerdos-México. On the stability of the cuboid singlet $(S_2)_4$ supermolecule: Benchmark ab initio studies. |
| *2013* | Talk. Science faculty of the Autonomous University of the Morelos state. April 12 Cuernavaca-México. On the stability of the cuboid singlet $(S_2)_4$ supermolecule: Benchmark ab initio studies |

*2013* Poster. MSSC2013-Ab *initio* Modeling in Solid State Chemistry. Summer Shool september 1-5 Turin-Italy. Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic.

*2013* Assistent. WSSQC-13. Workshop in Solid State Quantum Chemistry. septiembre 6-7 Turin-Italia.

*2013* Talk. XII Mexican meeting of theoretical physical chemistry. November 13-16 Querétaro-México. Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic.

*2014* Talk. Science faculty of the Autonomous University of the Morelos state. March 21 Cuernavaca-México. Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic.

*2014* Poster. International Meeting On Photodynamics and related aspects. October 26-31 Oaxaca-México. Understanding the $\varepsilon \rightarrow \zeta$ phase transition of solid oxygen. Periodic HF and Density Functional Theory studies with localized atomic basis.

*2014* Poster. XIII Mexican meeting of theoretical physical chemistry. November 5-8 Morelia-México. Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic.

*2015* Talk. 8th Workshop on condensed and molecular matter. June 12-15 Cuernavaca-México. Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic

*2015* Talk. National Autonomous University of Mexico. April 30 Cuernavaca-México. Talk: Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic

*2016* Talk. EAFIT University. May 26 Medellín-Colombia .Talk: Theoretical studies of oxygen at high pressures: phases $\varepsilon$ diamagnetic and $\zeta$ metallic

*2017* Talk. EAFIT University. February 22 Medellín-Colombia. Antiferromagnetic vs. non-magnetic $\varepsilon$ phase of solid oxygen. Periodic density functional theory studies using a localized atomic basis set and the role of exact exchange

*2018* Talk. Metropolitan Autonomous University. Quantum capacitance of graphene. February 16 Ciudad de México-México.

## JURY MEMBER OF MASTER THESIS

*November 2016* **Work evaluated:** Computational simulation of the structural and electronic properties of the molybdenum carbide (MoC) .

**Student:** Hernando Pérez Rave
**Advisor:** Dr. Jorge León David Caro
*EAFIT University*

*November 2017* **Work evaluated:** Contribution of magnetic ordering to the stability and electronic structure of the chrome nitride (CrN).

**Student:** Marco Marín Suárez
**Advisor:** MSc. Mario Elkin Vélez Ruiz
*EAFIT University*

PUBLICATIONS

Ochoa-Calle, A. J., R. Hernández-Lamoneda, and A. Ramírez-Solís (2013). "On the stability of the cuboid singlet (S2)4 supermolecule: Benchmark ab initio studies". In: *The Journal of Chemical Physics* 138.9, p. 094317. DOI: 10.1063/1.4793310.

Ochoa-Calle, A.J. and A. Ramírez-Solís (2014). "On the stability of the cyclic {O8} molecule". In: *Chemical Physics Letters* 592, pp. 326 –329. ISSN: 0009-2614. DOI: http://dx.doi.org/10.1016/j.cplett.2013.12.056.

Ochoa-Calle, A. J., C. M. Zicovich-Wilson, and A. Ramírez-Solís (2015). "On the Raman and infrared vibrational spectra of the $\varepsilon$ and $\zeta$ phases of oxygen. Systematic {DFT} studies with localized basis sets". In: *Chemical Physics Letters* 638, pp. 82 –86. ISSN: 0009-2614. DOI: http://dx.doi.org/10.1016/j.cplett.2015.08.036.

Ochoa-Calle, A. J. et al. (2015). "Understanding the $\varepsilon$ and $\zeta$ High-Pressure Solid Phases of Oxygen. Systematic Periodic Density Functional Theory Studies Using Localized Atomic Basis". In: *Journal of Chemical Theory and Computation* 11.3, pp. 1195–1205. DOI: 10.1021/acs.jctc.5b00017.

Ochoa-Calle, A. J., C. M. Zicovich-Wilson, and A. Ramírez-Solís (2015). "Solid oxygen $\zeta$ phase and its transition from $\varepsilon$ phase at extremely high pressure: A first-principles analysis". In: *Phys. Rev. B* 92 (8), p. 085148. DOI: 10.1103/PhysRevB.92.085148.

Ramirez-Solis, A., C. M. Zicovich-Wilson, and A. J. Ochoa-Calle (2017). "Antiferromagnetic vs. non-magnetic $\varepsilon$ phase of solid oxygen. Periodic density functional theory studies using a localized atomic basis set and the role of exact exchange". In: *Phys. Chem. Chem. Phys.* 19 (4), pp. 2826–2833. DOI: 10.1039/C6CP07445F.

Ramírez-Solís, Alejandro, Alvaro Jesús Ochoa-Calle, and Ramón Hernández-Lamoneda (2018). "Core excitations of the solid oxygen $\epsilon$ phase: periodic hybrid density functional theory studies with localized atomic basis". In: *Theoretical Chemistry Accounts* 137.3, p. 32. ISSN: 1432-2234. DOI: 10.1007/s00214-018-2213-4.

Ochoa-Calle, A. J. and M. Galvan-Espinosa. "Theoretical study of the quantum capacitance in graphene". In: *In preparation*.

THE THREE LETTERS OF REFERENCE HAVE BEEN SENT FOR YOUR CONSIDERATION.

Sincerely yours,

Álvaro de Jesús Ochoa Calle

May 18, 2018