
Curriculum Vitae

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PhD Physics

José A. Flores Livas
Oberwilerstrasse 124
CH-Basel 4054
Switzerland
+41 76-380-2721
jflores.livas@gmail.com
<http://www.fysik-aztek.net>

1.- Personal Information

I was born in San Pedro Coahuila, México in December 27th of 1985.

H-index: **13**. Average citation of **27**. More than **800** citations (ISI Web of Science).

Other: Google scholar ([link](#)). Researchgate ([link](#)) and ORCID: 0000-0002-4183-1316.

2.- Education

2009 - 2012 Ph.D in Physics, Université Claude Bernard Lyon 1, Laboratoire de Physique de la Matière Condensée. Lyon, France. Advisors: Prof. Miguel. A. L. Marques (theory) and Dr. Stephane Pailhes (experimental). Entitled: “*Computational and experimental studies of sp^3 -materials at high pressure*”. [Defended on September 19th 2012](#). [Committee: Prof. X. Gonze, Prof. A. Romero](#). [1]

2007 - 2008 Master in Physics, Universidad Autónoma de Nuevo León, Monterrey, México. Advisors: Prof. Eduardo Perez-Tijerina (experimental) and Prof. Sergio Mejia (theory). Entitled: “*Structure determination of AuPd icosahedral nanoparticles: experimental and computational studies*”. [Defended on June 13th 2008](#). [Committee: Prof. Juan Luis Chapa](#).

2002 - 2007 Bachelor studies in Physics, Universidad Autónoma de Nuevo León, Monterrey, México. Record: 87 /100.

[1] French system of Public Universities not longer confer levels of Latin honors, or degrees for dissertations such as “*summa cum laude*”. Rather they provide a detailed description of both, the defense (oral) and the overall PhD work. This document is used as qualification and serves to interpret the candidate’s success. You can read mine here: [Rapport-Soutenance Flores-Livas](#) (French). An official translation of this document in Italian is also available “[Rapporto PhD defense](#)”.

3.- Research Experience

- Sept. 2017 – Currently** Postdoc with MARVEL funds for my research at UniBas (CH).
- May 2015 – Aug. 2017** Postdoc in Prof. Goedecker’s group at UniBas (CH).
- Jan. 2013 – April 2015** Marie Curie scholarship, Max-Planck-Institute, Prof. E. K. U. Gross (DE).
- Oct. 2012 – Dec. 2012** Postdoc, University of Lyon 1, Prof. Marques (FR).
- March 2012** Experiments of Raman scattering on superconductors under pressure and very low temperature at ENS, Paris 6 (FR).
- April 2011** ARPES measurements in synchrotron Soleil, Cassiopée beamline (FR).
- December 2009** Neutron scattering measurements Orphee reactor CEA, Saclay (FR).
- September 2009** Started PhD (with my own scholarship from CONACyT Mexico) at the Université de Lyon 1, Prof. Marques and Dr. Pailhes (FR).
- June 2008 – Aug. 2009** Researcher in CIIDIT-UANL México (permanent position). I developed experimental tools: atomic layer deposition (ALD) chamber (MX).
- July 2007 – Dec. 2007** Scientific internship, synthesizing zeolites in thermochemistry lab (MX).
- June 2007 – July 2007** Summer internship at CINVESTAV. Synthesizing photovoltaic cells (MX).

4.- Co-supervising Junior Researchers

- **Miglė Graužinytė** (3 year PhD student UniBasel).

She completed her undergraduate and Master studies in Physics at the University of Edinburgh. Her research focuses on computational modelling of defects in semiconducting oxides. Since 3 years I am supervising and supporting her on the collaboration with experimental group (PVIab @ EPFL-Neuchatel).

- **Deb Sankar De** (3 year PhD student UniBasel).

Completed his master at Jawaharlal Nehru University (J.N.U), New Delhi. I am supervising his research since 2 and half years on clusters (fullerenes) for hydrogen storage and reconstruction of 2D materials for superconductivity.

- **Matheus Rodriguez Alvarez** (1st year PhD student Uni-Halle, Germany)

He is developing computational tools based on evolutionary algorithms to “reverse engineer” the electronic structure and design novel materials. I am supervising his work on intercalated- lanthanides for magnetism and support in coding, computing, etc.

5.- Teaching (Summary)

- Tutoring courses (exercise problem & solution), computational physics, statistical thermodynamics, electrodynamics, Monte Carlo methods for physics and fortran.
September 2015 to date, each semester alternating depending on the year, at University of Basel.
- Hands-out in density-functional theory (DFT) and magnetism, day 1 (compiling and basic ground state calculation) and day 2 (Magnetisms) with the “Elk code”.
Sept. 3 and 4, 2018 (15:00-17:00) at Max-Planck for Microstructure Physics Halle, Germany
- Taught density-functional theory (DFT) and hands on session day 1 (compiling and basic ground state calculation) and day 2 (Magnetism and relativistic calculations) in the “Electronic structure at the cutting edge with the Elk code”
August 10, 2015 to August 14, 2015 at CECAM-EPFL, Lausanne, Switzerland
- One semester teaching laboratory courses (experimental) 80 hrs. Subjects: fundamental physics (First year of BS), electromagnetism (Second year of BS) and digital-circuits (3 year of engineering).
2008 - 2009 at faculty of Physics of the UANL, Monterrey, Mexico.
- I gave a course on “Atomic force microscopy: introduction, theory and hands-on” at the International Workshop of Nanoscience-division of Mexican Society of Physics.
May 2009, duration: 8 hours in Mexico.

6.- Approved Research Projects

- **Computing grant** in Leibniz Supercomputing Centre (**LRZ**) of the Bavarian Academy of Sciences. More than 2.6 millions of CPU (SuperMUC) for 4 years. Germany (2018).
- **Computing grant** in the National supercomputer **CSCS-ETH** granted me more than 800,000 computing node hours in (Piz Daint) for a period of 2 years. Switzerland (2017).
- Project “ExMaMa” **EU Marie-Curie** of 161,968.80 Euro for 2 years- EU-IEF 329386 (2013).
- **PhD project** found by **CONACyT** with 35,000 Euro for 3 years. Number: 212868 (2009).

7.- Presentations, invited talks, seminars and keynotes (32)

- Contributed talk: “Emergence of hidden phases of methylammonium lead-iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) upon compression” presented in the International Workshop on Computational Design and Discovery of Novel Materials, COMDI MARVEL, *Sept. 10, 2018 EPFL-CH, Sept. 10, 2018*
- **Invited talk:** **Workshop on Electronic Structure methods: ELK Code**, Max-Planck Halle, “**Structure Prediction Algorithms: In Silico Design of Materials**”, *Germany, Sept. 6, 2018*
- **Invited talk:** **International Workshop on Electronic Structure of Superconductors & Novel Materials, Sapienza Universita di Roma**, “**Superconductivity in doped hydrides at high pressure**” ([link](#)). *Italy, May 24, 2018*
- Oral contribution: “Novel Rare-Earth Magnetic Nitride Perovskites” at the American Physical Society meeting. *USA, March 7, 2018*
- Seminar: in NanoPhononics group UniBas “Designing Quantum Materials” *Feb. 5, 2018*
- **Invited Seminar:** **MARVEL Junior Seminar Series “Computational screening of useful hole-electron dopants in SnO_2 ”**. *Switzerland, November 9, 2017*
- **Invited talk:** **652 WE-Heraeus “Ab initio Electronic Structure Theory in the 21st Century”** ([link](#)). *Germany, October 2017*
- Flash and highlighted presentation: “Interplay between structure metastability & superconductivity in elemental P” at the MARVEL retreat. *Switzerland, September 2017*
- **Invited Keynote:** “**Cutting edge structure prediction methods and in silico materials design**” **YRM-2017** ([link](#)). *ETSF Spain, June 2017*
- Flash and highlighted presentation: “Computational design of novel sulfide-type superconductors” MARVEL retreat, *Switzerland, April 2017*
- **Invited talk:** “**Fully ab-initio description and prediction of novel materials under high pressure**” *SMEC conference, USA, April 2017*
- **Invited Seminar:** **presenting in the group of Prof. Umrigar at Cornell University. “Doped ice under pressure”** *USA, March 28th, 2017*
- Oral contribution: “Emergence of superconductivity in H_2O ” at the American Physical Society (APS). *USA, March 2017*
- Oral contribution: “Emergence of superconductivity in ice at high pressure” at TRNM IX Program <http://trnm.aalto.fi/>. *Finland (2017)*
- **Seminar:** “**Emergence of superconductivity in ice at high pressure**”. **Atomistic seminar series in the Chemistry Department of University of Basel**. *Switzerland, Sept. 19, 2016*
- Presentation in the 2nd. review of MARVEL project about my research in hydrogen compounds under pressure. *Switzerland, April 2016*
- Oral contribution: “Superconductivity in metastable phases of P-H compounds” at the American Physical Society (APS). *USA, March 2016*
- Oral contribution: “Superconductivity in intercalated group-IV honeycomb structures” at the DPG-Frühjahrstagungen. *Germany, 2015*
- Oral contribution: “Computational search for rare-earth-free hard-magnetic materials” at the DPG-Frühjahrstagungen. *Germany, 2015*
- Oral contribution: “Computational search for rare-earth-free hard-magnetic materials” at the American Physical Society (APS). *USA, March 2015*

- Oral contribution: “Computational search for energy materials: rare-earth-free hard-magnetic materials.” at TRNM VIII. *Finland 2015*
- **Invited Seminar:** “Computational search for rare-earth-free hard-magnetic materials” in **Prof. Gohda’s Tokyo Institute of Technology.** *Japan, January 20, 2015*
- **Invited Seminar:** “Crystal prediction: Novel hard-magnetic materials” at **University of Basel, Prof. Goedecker.** *Switzerland, November 27, 2014.*
- Oral contribution: “Phonon-driven superconductivity in group-IV layered superconductors” at the EHPR Meeting. *France. 7-12 September 2014*
- Oral contribution: “High-throughput computational search for bulk materials with an enhanced MAE” at IMRC XXIII. *Mexico, August 2014*
- Oral contribution: “High-throughput computational search for hard-magnetic materials: ExMaMa project” at the DPG-Frühjahrstagungen. *Germany, 2014*
- Talk: at CFCAM meeting on pseudopotentials. About my contribution to the Delta project (Science paper). *France, February 2014*
- **Invited talk:** “Designing new materials from first principles: Computational and experimental results.” **Abinit Workshop Developers 2013.** *France 2013*
- Talk: “First Principle Design of superhardmagntes” MPI-Cooperation between Dresden and Halle, held at Goslar. *Germany 2013*
- Oral contribution: “Enhancing the superconducting transition temperature of BaSi2 by structural tuning.” at IMRC XX. *Mexico 2011*
- Oral contribution: “Structure determination of AuPd Icosahedral nanoparticles from: Experimental to computational results.” at IMRC XVIII. *Mexico 2009*
- Oral contribution: “Structural and electrical properties of ZnO ultra-thin films deposited by atomic layer deposition.” at IMRC XVIII. *Mexico 2009*

8.- Scientific reviewing activities

Reviewer of 29 manuscripts for the following journals:

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|------------------------------------|---|
| ● Phys. Rev. X | ● The Journal of Physical Chemistry C |
| ● Annalen der Physik | ● The European Journal of Physics B |
| ● Nanoscale (RSC) | ● Inorganic Chemistry |
| ● Physics Letters A | ● Computational Materials Science |
| ● Journal Phys. Condens. Matter. | ● Carbon |
| ● Journal of Materials Chemistry C | ● PCCP (RSC) |
| ● Communications Chemistry | ● Other journals and reviewer of C.E.A. projects (France) |
| ● Scientific Reports | |

9.- Organisation of Conferences

1. Main coordinator of 2018 MARVEL Junior Retreat (EPFL).
Website: <https://sites.google.com/view/Marvel-Junior-Retreat-2018/participants>

10.- Awards

As an undergraduate and a grad, I was awarded more than **5** times for “best poster” presentation. As a bachelor student, I was frequently awarded for best grades as well as for designing apparatus and experiments.

I won 2 stipend sponsored by MRS (Materials Research Society, U.S.A.) to attend (including flight, hotel and allowance) the spring meeting of MRS in San Francisco.

Among other top-awards, I consider the following ones as the most important in my career:

- Best poster presentation in the MARVEL retreat Switzerland (*Sept. 2017*).
- Selected among thousands of candidates (worldwide) to attend the **66th Lindau Nobel Laureate Physics** meeting. A week with 30 Nobels laureates (I am Lindau alumni) (*2016*).
- Award for my project “ExMaMa” funds by EU Marie-Curie of 161,968.80 Euro (*2013*).
- Award of a **Max-Planck stipendium** for post-doctoral in group of Prof. E. K. U. Gross (*2012*).
- Second place in the best poster presentation contest at IMRC-XX, Cancún, México (*2011*).
- Award: Scholarship to attend the MRS spring meeting in San Francisco, USA (*2010*).
- Award of a **Scholarship of Excellence** by CONACyT-México to pursuit my Ph.D studies (National council for science). Only ~10 annual stipends are granted in México (*2009*).
- First place in the best poster presentation contest at IMRC-XVIII, Cancún, México (*2009*).
- Best poster presentation at the “First Symposium of Scientific Research and Technological Innovation” celebrated in CIIDIT México (I won my first laptop) (*2009*).
- First place at the best poster presentation contest at IMRC-XVII, Cancún, México (*2008*).
- First place for high performance grades, faculty of physics in Monterrey, Mexico (*2007*).
- First place in science fair at faculty of physics on category of experiments: development of an apparatus to measure the velocity of sound and its variation in temperature (*2006*).

11.- Outreach activities

I have been contributing to outreach activities over the last 9 years; explaining physics, science concepts and supercomputers to a wide variety of audiences. – this includes not just the creation and delivery of lectures and presentations, but also participating in much more informal and interactive discussions in different languages. To highlights some of them:

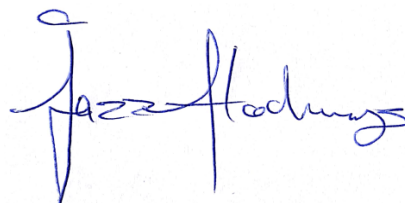
- TecDay by satw in Gymnasium Lerbermatt (Bern), 19. Oktober 2017 (in German).
- Lange Nacht der Wissenschaft Halle-Saale Max Planck Institute 2014 (in German).
- Radio interviewed talking about Science Monterrey, 2012 (in Spanish).
- Fête de la science, Campus de la Doua, Lyon 2011 (in French).
- Visit the DIF and talk about my experience of studying in europe 2010 (in Spanish).

12.- Poster presentations (+16)

- “Interplay between structure metastability and superconductivity in elemental P” at MARVEL retreat (**selected as best poster**). *Switzerland, Sept. 2017*
- “Machine learning for superconductors” at MARVEL 3rd review. *Switzerland, April 2017*
- “Hydrogen compounds under pressure” at MARVEL 2nd review. *Switzerland, April 2016*
- “Superconductivity of H₃S and H₃Se compounds” at PSI-K (2015). *USA, September 2015*
- “Phonon-mediated superconductivity in carbides, disilicides and germanides” at IMRC XXIII *Mexico 2014*
- “Magnetic anisotropy calculations” at Strong electron correlation effects in complex d- and f-based materials workshop, *Czech Republic, July 2014*
- “Hard magnets by computing design” at TRNM VII. [Program](#) *Finland, February 2014.*
- “Designing New Superhardmagnets from First Principles”. ELK workshop (summer school) at CECAM-EPFL. *Switzerland, July 2013*
- “Improving the electron-phonon interaction in layered disilicides” IMRC XX (**2nd place of best poster contest**). *Mexico, 2011*
- “Ab-initio calculations on thermoelectric properties of AEM-disilicides” G.D.R. de Thermoélectricité at Université Paris-Sud á Orsay. *France, July 2011*
- “Clathrates compounds under extreme conditions” Symposium W. (MRS) Spring Meeting in San Francisco. *USA, 2010*
- “Self assembling growth of ZnO ultra thin films by atomic layer deposition” at IMRC XVIII (**1st place of best poster contest**). *Mexico, 2009*
- “AuPd nanoparticles from: experiment to computational results” 1st Symposium of CIIDIT (**1st place of best poster contest**). *Mexico, 2009*
- “Gold/palladium nanoparticles in flight thermal annealing. (MRS) Spring Meeting. *USA, 2009*
- “Morphological studies of AuPd-nanoparticles” at IMRC XVII (**1st place of best poster contest**). *Mexico, 2008*
- “First stages of CdTe thin film deposit by CSVT.” XXVII Mexican Material and surfaces. *Mexico, 2007*

13.- Languages

- **English** +550 points in TOEFL (certified).
- **French** level tested C1 (certified).
- **German** B1 (certified).
- **Italian** B2 (certified).
- **Spanish** (Castilian) mother language.



*I declare the authenticity of the CV and that
all the information provided is correct.*