

CURRICULUM VITAE ABREVIADO (CVA)

Last 5 years: 2020 - 2024

A. PERSONAL INFORMATION

CV date 2024/22/11

First name	Aritz		
Family name	Leonardo Liceranzu		
e-mail	aritz.leonardo@ehu.eus	URL web	https://aritz.bcb.eus/
ID number		Age	45
Open Researcher and Contributor ID	Researcher ID	AAA-9337-2019	
	ORCID	https://orcid.org/0000-0002-5942-2270	

A.1. Current position

Position	Associate professor at Univ. of the Basque Country & associate researcher at Donostia International Physics Center		
Faculty	Science and Technology		
Department	Physics		
Address	Sarriena s/n LEIOA		
Phone	946015338	Research URL	https://bcb.eus/
Position category	Associate professor		
Key Words	Many body response functions; Electronic and magnetic properties in solids; Vibrational properties and Anharmonicity; Superconductivity; High Pressure; Biophysics; Molecular dynamics; Machine Learning; Deep Learning		

A.2. Education

PhD, Licensed, Graduate	University/Country	Year
Licensed in Physics	EHU-UPV/Spain	2003
PhD in Physics (Cum Laude)	EHU-UPV/Spain	2008
"Electron-phonon interaction in metals and inelastic effects in quantum well resonators" (Cum Laude)		

A.3. Previous positions (research activity interruptions, indicate total months)

Position	Center	Dates
Associate Professor	UPV-EHU	02/2020 - today
Lecturer	UPV-EHU	09/2017 - 01/2020
Lecturer	UPV-EHU	09/2012 - 08/2017
Postdoctoral Fellow	ESS-Bilbao	01/2010 - 08/2012
Postdoctoral Fellow	University of Missouri	01/2009 - 10/2010
Researcher	Gerdau (Sidenor I+D)	02/2008 - 01/2009
PhD student	Donostia International Physics Center	09/2003 - 02/2008

A.3. JCR articles, h Index, thesis supervised...

- 33 JCR articles
- six-years periods recognised by ANECA: 2 (last one in 2021)
- PhD supervised: 2 already defended and 2 in progress.
- Total number of citations to date: 550
- h index: 13

B. CV SUMMARY (*max. 5000 characters, including spaces*)

I graduated in Physics from the University of the Basque Country in 2003. Subsequently, I obtained a predoctoral scholarship to carry out my thesis in the field of condensed matter physics at the Donostia International Physics Center (DIPC), under the supervision of professors Eugene Chulkov and Pedro Miguel Echenique. The main task of my thesis was to ab initio evaluate the contribution of the electron-phonon interaction to the lifetime of electronic states using a calculation method we developed.

Upon completing my thesis, I joined the research team at SIDENOR I+D, a steel company specializing in high-performance special steels. There, I led the assembly and development of a high-frequency ultrasound machine to detect microscopic impurities in steels used for bearings. This system, still in use, improves the characterization of special steels for manufacturing decisions.

Later, I decided to return to the academic field and obtained a two-year postdoctoral contract at the University of Missouri, under the supervision of Professor Carsten Ullrich. I developed a method to directly calculate excitonic energies in semiconductors, ab initio solving the Casida equations without explicitly calculating the material's response function. This led to numerous publications within the group.

My career path led me to secure a permanent researcher position at ESS-Bilbao, within the Accelerator Physics department, where I collaborated with CERN on the design of electromagnetic cavities and beam simulations for the proton linear accelerator that will be part of the future neutron spallation source ESS-Lund.

Since 2012, I have been a professor in the Physics department at the University of the Basque Country. During these years, I have taught undergraduate courses such as General Physics, Mechanics, and Waves, as well as Topics in Fundamental Physics in the Master's program in Science and Quantum Technologies. Additionally, I have supervised 18 undergraduate projects, 4 master's projects, and 2 doctoral theses. In terms of scientific management and outreach, I served as coordinator for the Physics degrees and the double degree in Physics – Electronic Engineering for 2 years, and currently, I am a secretary of an admissions board for UPV-EHU and coordinator of the Physics booth during Science Week.

Currently, I am pursuing two lines of research:

- a) **Condensed Matter / Materials Science**. Electronic excitations in semiconductors (TDDFT) and Magnetism and topological transitions in 2D materials.
- b) **Computational Biophysics and Bioinformatics**. In 2019, together with Professor Aitor Bergara, I founded "Bilbao Computational Biophysics," where we investigate: Co-translational protein folding: forces and mutations, Machine Learning models to estimate the clinical impact of known mutations in channels, and drug design.

C. RELEVANT MERITS

C.1. Publications (last 5 years)

1. Light-induced reorientation transition in an antiferromagnetic semiconductor
PRX accepted (2024)

2. Identification of Riluzole derivatives as novel calmodulin inhibitors with neuroprotective activity by a joint synthesis, biosensor, and computational guided strategy.
Biomedicine & Pharmacotherapy 174, 116602 (2024)

3. MLe-KCNQ2: An Artificial Intelligence Model for the Prognosis of Missense KCNQ2 Gene Variants
International Journal of Molecular Sciences 25 (5), 2910 (2024)

4. Wigner-Seitz truncated time-dependent density functional theory approach for the calculation of exciton binding energies in solids.
Physical Review B 108 (23), 235210 (2023)

5. Molecular dynamics simulations of the calmodulin-induced α -helix in the SK2 calcium-gated potassium ion channel

Journal of Biological Chemistry 299 (2) (2023)

6. Magnetic order and magnetic anisotropy in two-dimensional ilmenenes

Nanoscale Advances 5 (10), 2813-2819 (2023)

7. Magnons and magnetic fluctuations in atomically thin MnBi_2Te_4

Nature Communications 13 (1), 2527 (2022)

8. Light-driven topological and magnetic phase transitions in thin layer antiferromagnets

The Journal of Physical Chemistry Letters 13 (18), 4152-4158 (2022)

9. Out-of-plane magnetic anisotropy in bulk ilmenite CoTiO_3

Physical Review B 105 (14), 144425 (2022)

10. Do calmodulin binding IQ motifs have built-in capping domains?

Protein Science 30 (10), 2029-2041 (2021)

11. Electron-Phonon and Spin-Lattice Coupling in Atomically Thin Layers of MnBi_2Te_4

NANO LETTERS 21, 14, 6139-6145 (2021)

12. $\beta\text{-As}_2\text{Te}_3$: Pressure-induced three-dimensional Dirac semimetal with ultralow room-pressure lattice thermal conductivity

Physical Review B 104 (2), 024103 (2021)

13. An epilepsy-causing mutation leads to co-translational misfolding of the Kv7. 2 channel

BMC biology 19 (1), 109 (2021)

14. Phonon-mediated dimensional crossover in bilayer CrI_3

Physical Review B 102 (8), 081117 (2020)

15. Group theory study of the vibrational modes and magnetic order in the topological antiferromagnet MnBi_2Te_4

Physical Review B 102 (10), 104102 (2020)

2025 (submitted articles in review):

1. 2-Acyl Pyrrole Derivatives as Novel Anti-Leishmanial Drug Candidates: Target Prediction, and Compound Optimization.

Journal of Medicinal Chemistry

2. A machine learning-based approach to predict drug-like molecules targeting Calmodulin pathway proteins.

Nature machine intelligence

3. Long-lived Zone-boundary Magnons in an Antiferromagnet

Nature Communications

4. Magnetic Order and Strain in Hexagonal Manganese Pnictide CaMn_2Bi_2

<https://arxiv.org/abs/2410.23053>

5. Structural Plasticity of Trigger Factor and its Role in Co-Translational Folding: Insights from High-Speed Atomic Force Microscopy and Molecular Dynamics Simulations

Nature Structural & Molecular Biology

C.2. Congress, indicating the modality of their participation (invited conference, oral presentation, poster) (last 5 years)

Title: Improved KCNQ2 genemissense variant interpretation with artificial intelligence

Type of participation: ORAL

Conference: American Physical Society March Meeting 2024

Abstract: <https://meetings.aps.org/Meeting/MAR24/Session/F18.8>

Place: Minneapolis

Date: 2024/05/03

Title: Layer-dependent phonons in the magnetic topological insulator MnBi_2Te_4

Type of participation: ORAL

Conference: American Physical Society March Meeting 2021

Abstract: <https://meetings.aps.org/Meeting/MAR21/Session/L52.7>

Place: virtual due to COVID

Fecha: 2021/17/03

Title: Phonon-mediated magnetic order control of bilayer antiferromagnets

Type of participation: ORAL

Conference: American Physical Society March Meeting 2020

Abstract: <https://meetings.aps.org/Meeting/MAR20/Session/W47.7>

Place: virtual due to COVID

Date: 2020/06/03

C.3. Research projects, indicating your personal contribution. In the case of young researchers, indicate lines of research for which they have been responsible. (last 5 years)

Title of the project: iFATALS: Desarrollo de una Terapia Novedosa de la ELA mediante la Regulación del Metabolismo Lipídico

Financing entity: Basque Government RIS3 (Health Department). Ayudas a proyectos de investigación y desarrollo en salud 2024: Potenciación de la investigación en salud de carácter estratégico.

Grant awarded: 99.220 €

Start date: 2024/01/12

Finish date 2026/01/12

PI: Aritz Leonardo Liceranzu (EHU and DIPC)

Title of the project: Exploring the interaction of electronic and dynamic excitations in nanostructures and complex systems

Financing entity: Ministry of Science and Innovation (PID2022-139230NB-I00)

Grant awarded: 137.500 €

Start date: 2023/01/12

Finish date 2026/01/12

PI: Andrés Ayuela (CSIC)

Title of the project: From protein folding prediction to personalized medicine with artificial intelligence

Financing entity: Basque government (IT-1707-22)

Grant awarded: 112.000 €

Start date: 2022/1/1

Finish date 2025/1/1

PI: Aitor Bergara (DIPC-EHU)

Title of the project: Photonic concrete for environmental solutions

Financing entity: Ministry of Science and Innovation (TED2021-132074B-C32)

Grant awarded: 130.400 €

Start date: 2022/1/12

Finish date 2023/1/12

PI: Andrés Ayuela (CSIC)

Title of the project: Electron Excitations and Dynamics in Surfaces and Nanostructures (3EDDiSNa)

Financing entity: Ministry of Science and Innovation (PID2019-105488GB-I00)

Grant awarded: 161.000 €

Start date: 01-06-2020

Finish date 30-05-2023

PI: Andrés Ayuela (CSIC) and Vyacheslav M. Silkin

Title of the project: Grupo de Biofísica Teórica y Aplicada de Proteínas

Financing entity: UPV-EHU (GIU18/172)

Grant awarded: 25.470 €

Start date: 01-01-2019

Finish date 12-31-2021

PI: D.M. Guerín (UPV/EHU)

Title of the project: Versatile integrated platform for the development of new disease treatments (CardiCaM)

Financing entity: ELKARTEK – SPRI Basque government

Grant awarded: 480.126 €

Start date: 2020/1/1

Finish date 2021/31/12

PI: Álvaro Villarroel (CSIC)

C.4. Participation in technology/knowledge transfer activities and results exploitation Include patents and other industrial or intellectual property activities (contracts, licenses, agreements, etc.) in which you have collaborated.

- **Founder of BioComputing (2024):**

A startup created to support and accelerate the research of laboratories and industries by integrating computational methods into biological and engineering experiments.

Website: <https://biocomputing.es/>.

Contracts achieved:

- **GRIFOLS:** In-Silico antibody optimization (NDA signed). (18.000 €)
- **INNOPROT:** Design of nanobodies using AI to detect alpha-synuclein aggregates. (6.000 €)
- **MOLECULAR COGNITION LAB** (<https://shiraknafo.com/>): Machine Learning models applied to the Epitranscriptomic Signatures in Neurological Disorders Using m6A Modifications. (12.000 €)
- **AERNNOVA:** Cost predicting software (NDA signed). (12.000 €)