CURRICULUM VITAE ABREVIADO (CVA)

IMPORTANT – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.

Part A. PERSONAL INFORMATION

First name	Massimiliano		
Family name	Stengel		
Gender (*)	Male	Birth date (dd/mm/yyyy)	20/04/1974
Social Security, Passport, ID number	NIE: Y0364177D		
e-mail	mstengel@icmab.es	URL Web	
Open Researcher and Contributor ID (ORCID) (*)		0000-0003-4175-3888	

(*) Mandatory

A.1. Current position

Position	ICREA Research Professor		
Initial date	01/10/2011		
Institution	Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)		
Department/Center	Theory and simulation		
Country	Spain	Teleph. number	935 801853
Key words	first-principles; density-functional theory; linear response; ferroelectricity; flexoelectricity; piezoelectricity; multiferroics; thin films; interfaces; surfaces; 2D materials		

A.2. Previous positions (research activity interuptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
2010-2011	Ramón y Cajal fellow at ICMAB-CSIC (Spain)
2009 2005-2009 2000-2004	Postdoctoral fellow at CECAM (Switzerland) Postdoctoral fellow at UCSB (USA) PhD student at EPFL (Switzerland)

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Docteur és Sciences	Ecole Polytechnique Fédérale de Lausanne (Switzerland)	2004
Laurea in Fisica	Università degli Studi di Trieste	1999

(Include all the necessary rows)

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

Massimiliano Stengel's research specializes in the development of frontier first-principles simulation approaches, and in their application to materials science problems of fundamental and technological relevance. He has a strong record of methodological breakthroughs in first-principles theory that led to solving long-standing open questions in several areas:

Ferroelectricity. MS developed an innovative method to calculate capacitors under an applied bias (MS, N. Spaldin and D. Vanderbilt, Nature Physics 2009), and thereby addressed 45-year old puzzle about the suppressed performance (“dead layer effect”) of ultrathin devices (MS and N. Spaldin, Nature 2006; MS, D. Vanderbilt and N. Spaldin, Nature Materials 2009). These works had a remarkably large resonance, both at the level of invited presentations and citations.

Flexoelectricity, the coupling between the electrical polarization and a strain gradient, presents daunting technical challenges from the point of view of first-principles theory; these have thwarted direct calculation attempts for many years. MS overcame these difficulties and performed the first *ab initio* calculation of the full flexoelectric response of a real material, $SrTiO_3$ (MS, Nature Communications 2013; Phys. Rev. B 2013; Phys. Rev. B 2014). In 2016 he was awarded an ERC Consolidator Grant to pursue these studies, which culminated in a full-fledged code implementation (M. Royo and MS, Phys. Rev. X 2019; Phys. Rev. B 2022) of the bulk flexoelectric tensor in ABINIT. These methodological breakthroughs, initially motivated by flexoelectricity, opened many avenues for research in other unforeseen directions (some examples are described in the following).

Phonons and electron-phonon interactions. The methods developed in the context of flexoelectricity turned out to be valid, with minor changes, for a broad class of materials properties that depend on spatial dispersion. Among the latter, MS pioneered the calculation of dynamical quadrupoles, a higher-order multipolar counterpart of the Born effective charges. Dynamical quadrupoles were found to be important in the interpolation of the interatomic force constants (M. Royo, K. Hahn, MS, Phys. Rev. Lett. 2020) and electron-phonon matrix elements, both in 3D (Brunin et al., Phys. Rev. Lett. 2020) and 2D crystals (S. Poncé et al., Phys. Rev. Lett. 2023). More recently, he contributed to establishing a powerful adiabatic method to describe the coupled magnon/phonon dynamics (S. Ren et al., Phys. Rev. X, in press; J. Bonini et al., Phys. Rev. Lett. 2023), of immediate relevance for this project.

Optics. Another spatial dispersion effect, and probably the best known one, consists in the so-called natural optical activity. This is the property of some chiral crystals and molecules to rotate the plane of polarization of transmitted light. Very recently, MS pioneered (A. Zabalo and MS, Phys. Rev. Lett. 2023) a method to calculate the gyration coefficients in real materials with unprecedented accuracy and efficiency; the second part of this project is meant to build on this advance.

Two-dimensional (2D) materials. MS has targeted 2D materials on three main fronts. First, he established an exact framework to treat long-range electrostatic interactions and screening in 2D within a fundamental first-principles viewpoint (M. Royo and MS, Phys. Rev. X 2021); this achievement was key to the aforementioned electron-phonon study in 2D. Next, he addressed the problem of defining and calculating the flexoelectric response of 2D layers and membranes, overcoming earlier conceptual and technical difficulties in these regards (M. Springolo, M. Royo and MS, Phys. Rev. Lett. 2021; Phys. Rev. Lett. 2023). Note that flexoelectricity in 2D requires a specialized approach that builds upon (but significantly departs from) the established methods for 3D: additional terms need to be computed, which are crucial to obtaining a qualitatively correct physical picture. Finally, MS has recently led a pioneering study of flexomagnetism in bent CrI_3 monolayers (A. Edström et al. Phys. Rev. Lett. 2022).

In recognition of his innovative contributions and intense code development activity, MS was invited in 2022 to join the International Advisory Committee of ABINIT (https://www.abinit.org/advisory). He maintains a strong international network of collaborators, including X. Gonze (Louvain-la-Neuve, leader of the ABINIT project), D. Vanderbilt (Rutgers University), Nicola Marzari (EPFL), J. Iñiguez (LIST), Silvia Picozzi (CNR-SPIN) and Cyrus Dreyer (Stony Brook and Flatiron Institute). As of today, he has authored 78 publications, and has presented 48 invited talks at international conferences (including 5 at the APS March Meeting and 2 at the MRS Spring Meeting).

Part C. RELEVANT MERITS *(sorted by typology)*

C.1. Publications (selection of 10 publications in the last five years)

* Shang Ren, John Bonini, Massimiliano Stengel, Cyrus E. Dreyer, David Vanderbilt, *Adiabatic dynamics of coupled spins and phonons in magnetic insulators*, **Phys. Rev. X** (in press). Preprint at arXiv:2307.05668.

* Matteo Springolo, Miquel Royo, and Massimiliano Stengel, *In-Plane Flexoelectricity in Two-Dimensional D_{3d} Crystals*, **Phys. Rev. Lett**. 131, 236203 (2023)

* Asier Zabalo and Massimiliano Stengel, *Natural Optical Activity from Density-Functional Perturbation Theory*, **Phys. Rev. Lett.** 131, 086902 (2023)

* Samuel Poncé, Miquel Royo, Marco Gibertini, Nicola Marzari, and Massimiliano Stengel, *Accurate Prediction of Hall Mobilities in Two-Dimensional Materials through Gauge-Covariant Quadrupolar Contributions*, **Phys. Rev. Lett.** 130, 166301 (2023)

* Bonini, J.; Ren, S; Vanderbilt, D.; Stengel, M.; Dreyer, C. E.; Coh, S., *'Frequency splitting of chiral phonons from broken time.reversal symmetry in CrI3'*, **Physical Review Letters**, 130, 086701 (2023)

* Edström, A; Amoroso, D; Picozzi, S.; Barone, P.; Stengel, M., '*Curved magnetism in CrI_3*', **Physical Review Letters**, 128, 177202 (2022). (Editors' Suggestion.)

* Dreyer, CE; Coh, S; Stengel, M, '*Nonadiabatic Born Effective Charges in Metals and the Drude Weight*', **Physical Review Letters**, 128, 095901 (2022). (Editors' Suggestion.)

* Springolo, Matteo; Royo, Miquel; Stengel, Massimiliano, *'Direct and converse flexoelectricity in two-dimensional materials*', **Physical Review Letters**, 127, 216801 (2021).

* Royo, Miquel; Stengel, Massimiliano, *'Exact long-range dielectric screening and interatomic forces in quasi-2D crystals*', **Physical Review X**, 11, 041027 (2021).

* Royo, Miquel; Hahn, Konstanze R.; Stengel, Massimiliano, *'Using High Multipolar Orders to Reconstruct the Sound Velocity in Piezoelectrics from Lattice Dynamics'*, **Physical Review Letters**, 125, 217602 (2020).

C.2. Congress (selected invited talks at international conferences, last five years)

* *Flexoelectricity and flexomagnetism in two-dimensional materials*. CMD30 FisMat2023 joint conference (Milano, September 2023).

* *Flexoelectricity and long-range Coulomb interactions in two-dimensional crystals*. CMT@Brixen Workshop (Bressanone/Brixen, June 2023).

* *Flexoelectricity and long-range Coulomb interactions: from 3D to 2D*. 5th Anniversary Conference of CCQ (NYC, June 2022).

* *Flexoelectricity and long-range Coulomb interactions: from 3D to 2D*. 2022 Workshop on Recent Developments in Electronic Structure (ES22), Columbia University (NYC, June 2022).

* *Long-range dielectric screening and force constants in two dimensions*. ABINIT developer workshop (online, June 2021)

* *Long-range dielectric screening and force constants in two dimensions*. Total Energy Workshop (online, February 2021)

* *The bulk flexoelectric tensor from an ab initio perspective*. Fundamental physics of Ferroelectrics Workshop (online, January 2021).

* *First-principles theory of flexoelectricity and related materials properties*. Workshop on Total Energy and Force Methods, San Sebastian-Donostia (January 2000).

* *New functionalities from gradients: Flexoelectricity and more*. European Meeting on Ferroelectricity (EMF), Lausanne (July 2019)

* *New functionalities from gradients: Flexoelectricity and more*. International Workshop on Topological Structures in Ferroic Materials - TOPO2019, Prague (Czech Republic).

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

TITLE: Functional Oxide Single crystal Membranes (FOxMe)
FUNDING AGENGY: MICINN (proyectos I+D+i).
YEARS: 2020-2023.
PI: M. Stengel (PI of the ICMAB node) and G. Catalan.
BUDGET: 90,000 EUR for the ICMAB node

TITLE: Hierarchical multiscale modeling of flexoelectricity and related materials properties from first principles (MULTIFLEXO)
FUNDING AGENCY: ERC Consolidator Grant
YEARS: 2017-2023
PI: M. Stengel
BUDGET: 1,470,000 EUR

TITLE: Phase and Antiphase Boundaries and Domains in Antiferroelectrics (PHABADA)
FUNDING AGENGY: MINECO (proyectos I+D+i excelencia).
YEARS: 2016-2019.
PI: M. Stengel (PI of the ICMAB node) and G. Catalan (ICN2).
BUDGET: 50,000 EUR + 1 FPI Ph.D. fellowship for the ICMAB node

TITLE: Oxide stresstronics (OSTRES)
FUNDING AGENGY: MINECO (proyectos I+D+i excelencia).
YEARS: 2014-2017.
PI: M. Stengel (PI of the ICMAB node) and G. Catalan (ICN2).
BUDGET: 122,000 EUR + 1 FPI Ph.D. fellowship (22,000 EUR + 1 FPI for the ICMAB node)

TITLE: Fundamental studies and computational design of nanostr. multifunctional oxides.
FUNDING AGENGY: MICINN (proyectos de investigación fundamental no orientada).
YEARS: 2010-2013.
PI: Jorge Íñiguez (and involving M. Stengel and O. Diéguez as senior researchers).
BUDGET: 40,000 EUR

C.4. Contracts, technological or transfer merits, Include patents and other industrial or intellectual property activities (contracts, licenses, agreements, etc.) in which you have collaborated. Indicate: a) the order of signature of authors; b) reference; c) title; d) priority countries; e) date; f) Entity and companies that exploit the patent or similar information, if any

N/A