Curriculum Vitae

Personal Data

Title	Dr
First name	Dominique
Name	COSTA
Birth date	09/04/1962
Status	Married, one child
Current position	Research Director *(permanent position)*
Current institution(s)/site(s), country	Institut de Recherche Chimie Paris/Physico-Chimie des Surfaces
Identifiers/ORCID	*https://orcid.org/0000-0003-0236-9728*

D. Costa, aged 63, Researcher at CNRS, (120 publications, *h index* 46), is specialized in modelling with density functional theory (DFT) adsorption and reactions at metal and oxide surfaces.
She has specialized in modelling of passive films on stainless steels and aluminium and corrosion reactions thereon. She developed the DFT MD approach for metal-water and oxide-water interfaces.
She gave 50 talks, from which 8 invited conferences, and 17 invited seminars in French and European laboratories.

She was Host for the HPC-Supercomputing in Europe (12 visitors),
Member of the french GDR DFT++, GDR Mod-Mat.
She organized 3 meetings

Qualifications and Career *mixture of table/free text*

Stages	**Periods and Details**
Degree programme	***Material Sciences, 1984-1985, UPMC, France***
Doctorate	***March 1989, Supervisor: H Pezerat*** ***UPMC***
Stages of academic/professional career *(optional after doctorate)*	*Since 2016, Research Director at IRCP/PCS* *2007-2016: Researcher at Laboratoire de Physico-Chimie des Surfaces, Paris* *2004 : IFP invited researcher* *1996-2007 (except 2004) : Researcher at Laboratoire de réactivité de Surface, UPMC* *1990-1996 : Researcher at Laboratoire de Physico-Chimie de Surfaces*

The PCS modeling team has developed since ten years an atomistic approach of the corrosion phenomena, using Density Functional Theory (DFT) used to elucidate elementary events at the atomic scale. The passive film composition is determined at the molecular scale, as well as adsorption of corrosive/protective species or species for adhesion. An atomistic thermodynamics approach allows us to bridge the gap from the electronic calculations to experimental conditions

(*T, p*) and to propose predictive phase diagrams of stabilities of different terminations. DFT-MD (DFT Molecular Dynamics) is being applied to the interface metal/oxide/solvent.

Supplementary Career Information

I performed experimental science from my PhD to 1996, being familiar to XPS for corrosion science, then did a reconversion to theory (using mostly DFT), in the Lab. Reactivity of Surfaces. I was invited for one year at French Institute of Petroleum and worked exclusively on DFT, using VASP code. After that stay, I came back to the original lab Physico-Chemistry of Surfaces, to apply DFT to corrosion science.

Engagement in the Research System

Reviewer for peer-reviewed scientific journals (J. Phys. Chem., Langmuir, Surf. Science, Corrosion, Corrosion Science, Thin Solid Films, Soft Matter ; ~10 per year).
Member of IDRIS User's comity.
Member of French GENCI attribution CT8, Chemistry.
Member of Scientific Council IRCP/ENSCP, 2022-2024
Member of CNRS CAP, 2023-
Expert Referee for Slovenian Agency of Research 2024-
Member of HCERES, 2024
Member of French CNRS 14 commission, PEDR, 2018-2020

Supervision of Researchers in Early Career Phases

Supervision of 339 persons/months, (from which 74p/m post doctorates, 184p/m doctorates and 81p/m others)

Name	Grade	Begin-end	Subject	Collaboration
Minli Chen	PhD	2023-2026	Role of the oxide layer in the Hydrogen penetration in iron	IFPEN
Michaud M.	PhD	2023-2026	Discovery of universal corrosion inhibitors of Al alloys	PSL
Xian Huang	Post doc	2022-2024	Role of Mo in stainless steel corrosion inhibition	ERC CIMNAS
Lefevre J.	L3	March-June 2022	Implementation of python scripts for XPS quantitative analysis	U. Aix-Marseille
Costa S.	M2 stay (5 months)	2022	Artificial intelligence and music composition	IRCAM
Chiter Fatah	Post doc	2019-2020	Corrosion inhibition of Al alloys	M ERANET
Chiter Fatah	Post doc	2021-2023	Corrosion inhibition of Cu	ERC CIMNAS
Mirland A.	PhD	2021	XPS of Al alloys	PSL
Cantarelli C.	PhD	2021	Multi scale modelling of biofuel interaction with stainless steel and aluminium	IFPEN

Darenne B.	PhD	2017-2020	Multi scale modelling of biofuel interaction with stainless steel and aluminium	IFPEN
Vernack E.	PhD	2016-2019	Experimental and theoretical study of Cu and Al corrosion inhibition by MBT and MBI.	Socomore

Recent Scientific Results [1–11]

(1) Lê-Chesnais, J.; Steffenhagen, M.; Méthivier, C.; Costa, D.; Rodriguez, D.; Lambert, J.-F.; Maisonhaute, E.; Landoulsi, J. Binding Mechanism of Oligopeptides on Solid Surface: Assessing the Significance of Single-Molecule Approach. *Nanoscale* **2025**. https://doi.org/10.1039/D4NR04474F.

(2) Huang, X.; Costa, D.; Diawara, B.; Maurice, V.; Marcus, P. Protection of Stainless Steels by Mo against Cl Attack: A DFT Study. *J. Phys. Chem. C* **2025**, acs.jpcc.4c08056. https://doi.org/10.1021/acs.jpcc.4c08056.

(3) Huang, X.; Costa, D.; Diawara, B.; Maurice, V.; Marcus, P. DFT Study on Mo-Stabilized Passive Films: Hydroxylation Effects on Chromium and Iron Oxide Surfaces. *Corros. Sci.* **2024**, *233*, 112105. https://doi.org/10.1016/j.corsci.2024.112105.

(4) Huang, X.; Costa, D.; Diawara, B.; Maurice, V.; Marcus, P. Atomistic Insights on Enhanced Passivity: DFT Study of Substitutional Mo on Cr2O3 and Fe2O3 Surfaces. *Corros. Sci.* **2023**, *224*, 111543. https://doi.org/10.1016/j.corsci.2023.111543.

(5) Chiter, F.; Costa, D.; Poberžnik, M.; Milošev, I.; Marcus, P.; Kokalj, A. DFT Study of Cl − Ingress into Organic Self-Assembled Monol Ayers on Aluminum. *J. Electrochem. Soc.* **2023**, *170* (7), 071504. https://doi.org/10.1149/1945-7111/ace334.

(6) Chiter, F.; Costa, D.; Maurice, V.; Marcus, P. Corrosion Inhibition of Locally De-Passivated Surfaces by DFT Study of 2-Mercaptobenzothiazole on Copper. *NPJ Mater. Degrad.* **2021**, *5* (1). https://doi.org/10.1038/s41529-021-00198-x.

(7) Chiter, F.; Costa, D.; Maurice, V.; Marcus, P. Adsorption of 2-Mercaptobenzimidazole Corrosion Inhibitor on Copper: D FT Study on Model Oxidized Interfaces. *J. Electrochem. Soc.* **2020**, *167* (16), 161506. https://doi.org/10.1149/1945-7111/abcd4f.

(8) Milošev, I.; Zimerl, D.; Carriére, Ch.; Zanna, S.; Seyeux, A.; Iskra, J.; Stavber, S.; Chiter, F.; Poberžnik, M.; Costa, D.; Kokalj, A.; Marcus, P. Editors' Choice—The Effect of Anchor Group and Alkyl Backbone Chain on Performance of Organic Compounds as Corrosion Inhibitors for Aluminum Investigated Using an Integrative Experimental-Modeling Approach. *J. Electrochem. Soc.* **2020**, *167* (6), 061509. https://doi.org/10.1149/1945-7111/ab829d.

(9) Chiter, F.; Costa, D.; Maurice, V.; Marcus, P. DFT Investigation of 2-Mercaptobenzothiazole Adsorption on Model Oxidi Zed Copper Surfaces and Relationship with Corrosion Inhibition. *Appl. Surf. Sci.* **2021**, *537*, 147802. https://doi.org/10.1016/j.apsusc.2020.147802.

(10) Vernack, E.; Costa, D.; Tingaut, P.; Marcus, P. DFT Studies of 2-Mercaptobenzothiazole and 2-Mercaptobenzimidazole as Corrosion Inhibitors for Copper. *Corros. Sci.* **2020**, *174*, 108840. https://doi.org/10.1016/j.corsci.2020.108840.

(11) Vernack, E.; Zanna, S.; Seyeux, A.; Costa, D.; Chiter, F.; Tingaut, P.; Marcus, P. ToF-SIMS, XPS and DFT Study of the Adsorption of 2-Mercaptobenzothia-Zole on Copper in Neutral Aqueous Solution and Corrosion Protection in Chloride Solution. *Corros. Sci.* **2023**, *210*. https://doi.org/10.1016/j.corsci.2022.110854.