

# An Outline of My Activities

Mariano Forti

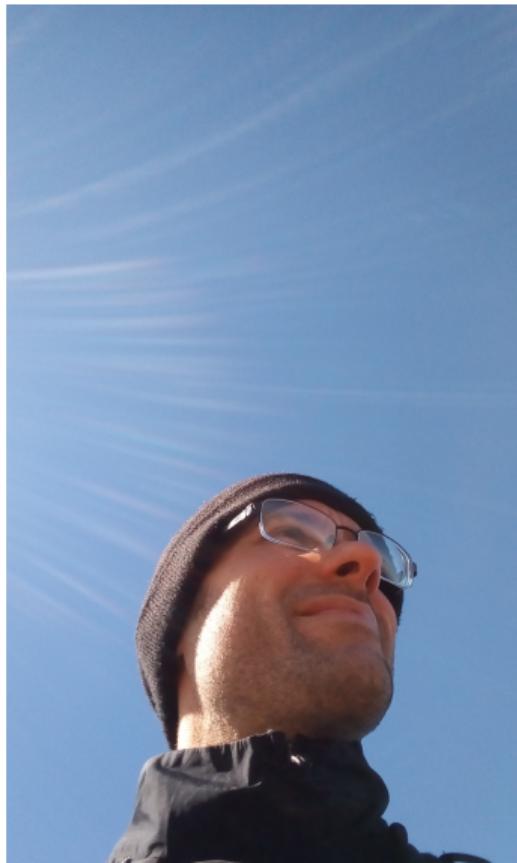
2019

[Interview details here](#)

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# Who am I

# Who am I?



## Current positions



Comisión Nacional  
de Energía Atómica



- Materials Engineer (2010), PhD Materials Science (2017)
- Wide Experience in DFT Calculations
- based at Argentina, Ciudad de Buenos Aires

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## Current Research

# Scientific support to Special Alloys Foundry

taking a small part since August 2018, but special challenge because this is strictly related to production of security related components of the CAREM reactor.

Standard and Technical documentation interpretation.

comparation of chemical analysis methods.

Quality assurance related stuff:

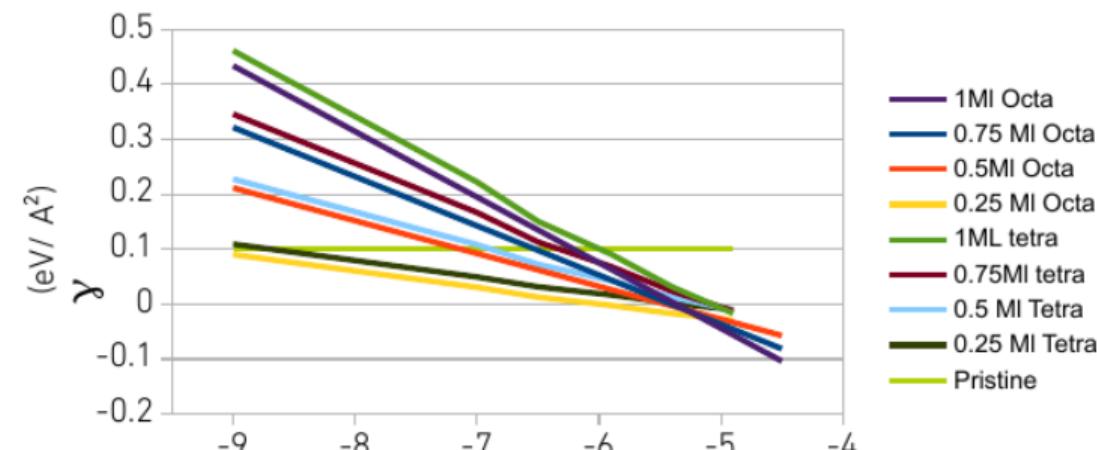
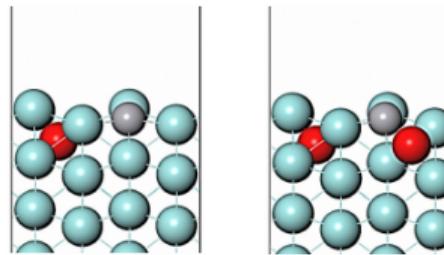
- documentation registries and archiving
- documentation codification

# Zr(10̄10) surface, Oxygen and Hydrogen Absorption

This project is carried on in collaboration with Fernando Soto, a Postdoc at Perla Balbuena's group in Texas A&M University, USA.

## Progress so far

- Oxygen Coverage with alloy elements

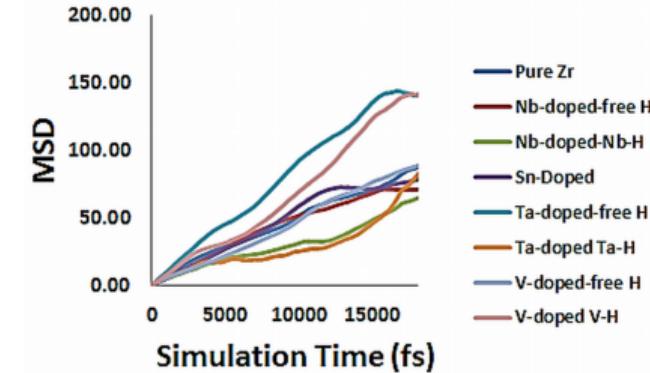
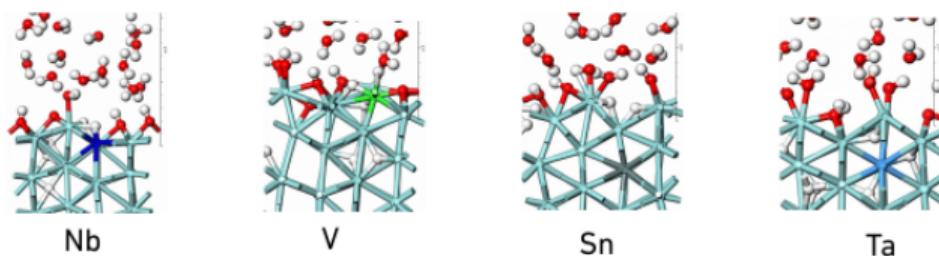


# Zr(10̄10) surface, Oxygen and Hydrogen Absorption

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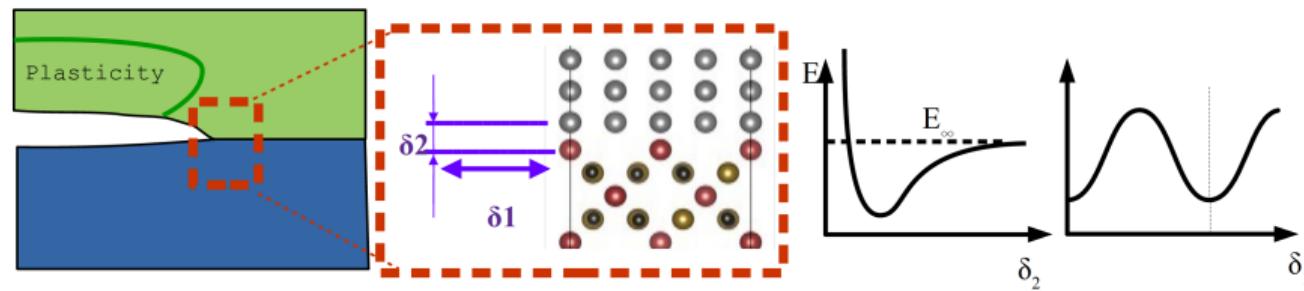
## Progress so far

- Oxygen Coverage with alloy elements
- AIMD: Hydrogen moves differently in the presence of Ta and V,

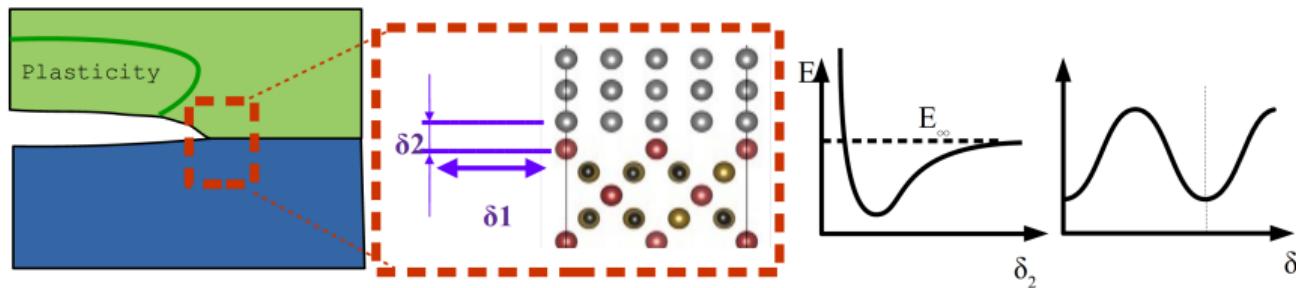


# Adhesion in FeBCC/Fe<sub>3</sub>O<sub>4</sub> interface

Separating the parts of the interface it is possible to obtain energy vs separation curves from DFT calculations. Then the forces can be obtained from interface potential models!



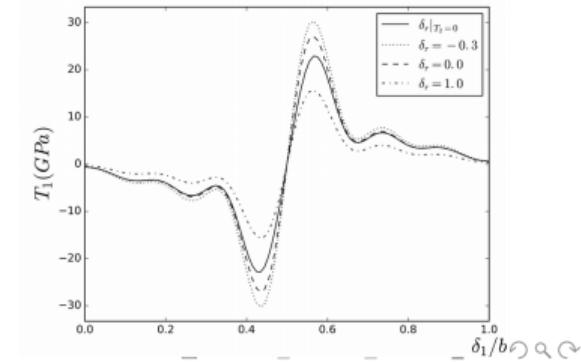
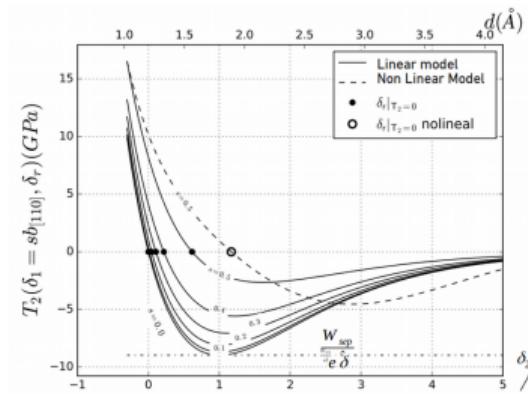
# Adhesion in FeBCC/Fe<sub>3</sub>O<sub>4</sub> interface



$$\tilde{L}_{\delta_1} = \frac{E_{ad}}{W_{sep}} = \exp\left(\frac{\delta_2}{\delta}\right) \sum_{i=0}^{i_{max}} (1+\beta)^i \left[ -1 + f(\delta_1) (1+\beta)^i \right] \alpha_i \left( \frac{\delta_2}{\delta} \right)^i$$

$$T_1(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_1}$$

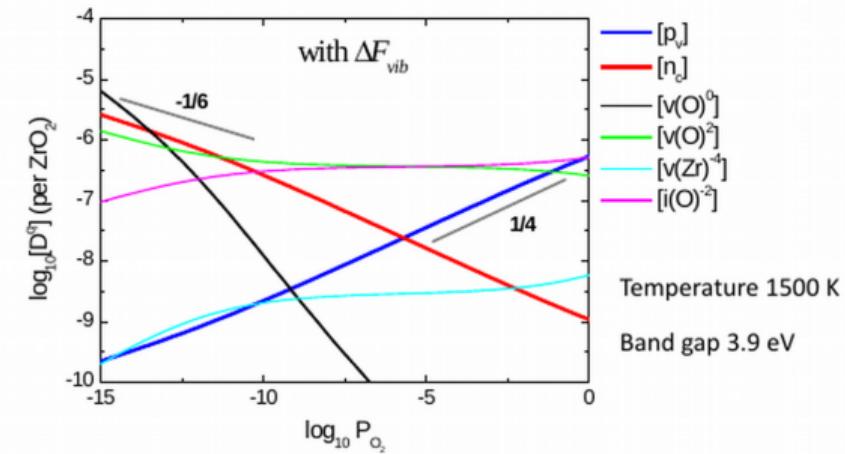
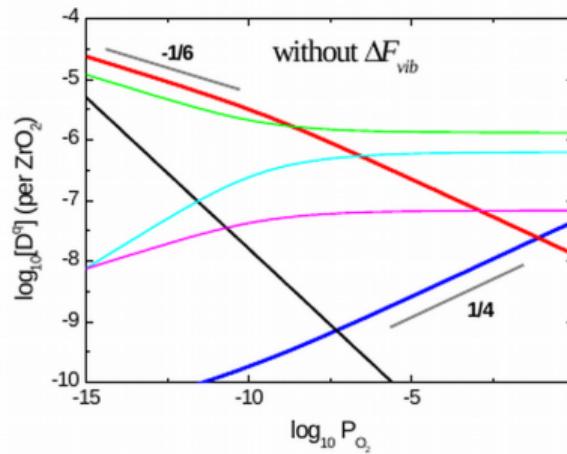
$$T_2(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_2}$$



# Point Defect Equilibria in tetragonal ZrO<sub>2</sub>

This Project is carried on in collaboration with Pablo Gargano and Gerardo Rubiolo from DAE. We performed DFT of Vibrational energies using a Debye Model.

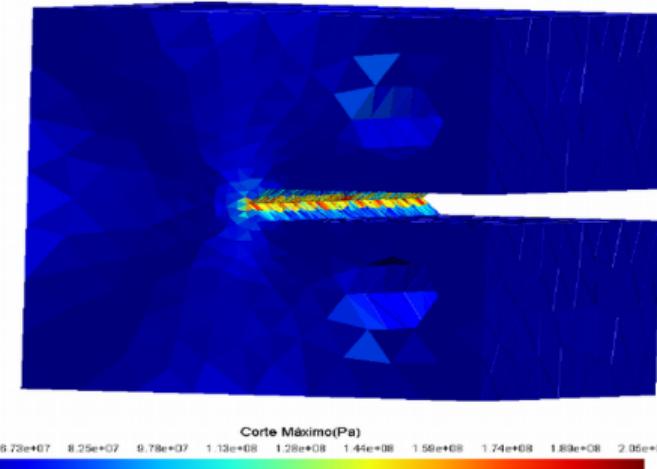
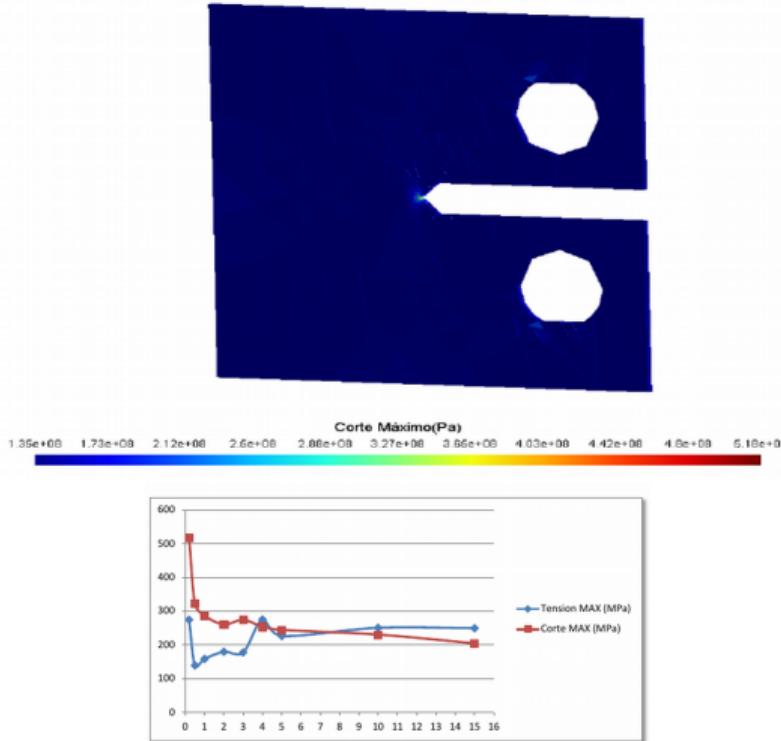
$$\Delta E_{D,q}^f = E_{tot}^{DFT}(D^q) - E_{tot}^{DFT}(\text{perfect}) - \Delta n_D \mu_D + q(E_{VBM} + \mu_F)$$



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# Teaching

# Teaching FEM basics



We guide students make while they build their own implementation of the Finite Element Method in any language they choose.

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## Other Skills

# Workflow and Programming

## ■ Programming, Mainly scripting

- Mainly Bash,
- FORTRAN
- Python
- matlab
- Couple Markup Languages (HTML, L<sup>A</sup>T<sub>E</sub>X Markdown)

## ■ Worflow Solutions, allways evolving

- bash, tmux and vim
- KDE
- local git repositories for versioning and history
- ssh, sftp
- Libreoffice and MSOffice

```

Izquierdo          Archivo      Utilidades      Opciones      Derecho
...                Nombre        Tamaño | fecha Modifi  [^]  ...                Nombre        Tamaño | fecha Modifi
/..               /..           /DIR-ANT
/Bitacoras        /Bitacoras   4996 sep 11 19:04  /..
/ComprobantesPago /ComprobantesPago 4996 jun 26 2017  /INPUTS
/Crack            /Crack       4996 ago 23 16:50  /z1_atdl
/CuadernoTrabajo /CuadernoTrabajo 4996 oct 1 17:15  /z2_atdl
/Desktop          /Desktop     4996 ago 16 16:37  /z3_atdl
/Devel             /Devel       20480 jun 26 2017  /z4_atdl
/Documents         /Documents   4996 sep 7 09:46  /z5_atdl
DIR-ANT
5944M/79G (7%)
sftp: Listado completo.
mariano@office:Bitacoras $ 1 Ayuda 2 Menú 3 Ver 4 Editar 5 Copiar 6 RenMov 7 Mkdir 8 Borrar 9 Menú 10 Salir
50
51 cd STD
52
53
54 FIXNPAR=1
55 CASE=CHG
56 AFTER=$CASE`dir
57 cp $SLURM_SUBMIT_DIR/*.sh .
58 USEINCAR=$SLURM_SUBMIT_DIR/INCARS/INCAR-$CASE
59 USEPOTCAR=$SLURM_SUBMIT_DIR/INPUTS/POTCAR
60 USEKPOINTS=$SLURM_SUBMIT_DIR/INPUTS/KPOINTS-TOTEN
61
62 runysave
63
64
65 cd $SLURM_SUBMIT_DIR
66
50,0-1 73%
moffice" 02:03 17-oct-18

```

Disclaimer: Image is only an illustration, does not represent my real workflow

# Linux Sysadmin

- Installation and maintenance of small Rocks Clusters
- Compilation and maintenance of VASP and other programs in this and other clusters.
- some basic file recovery with testdisk and scalpel



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## Conclusions

# Such Experience, Much promise

- Wide DFT experience gives me the tools to face all kind of difficult computational materials science problems
- Experience in programming and linux system administration can give me a good insight in everyday work
- experience in interacting in multidisciplinary workgroups.

Any Questions?

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