

# An Outline of My Activities

Mariano Forti

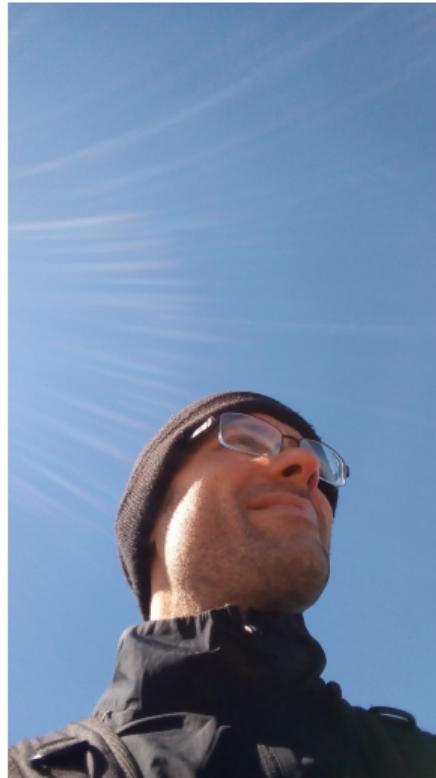
2019

[Interview details here](#)

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# Who am I

# Who am I?



## Current positions



Comisión Nacional  
de Energía Atómica

División Aleaciones Especiales



- 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.

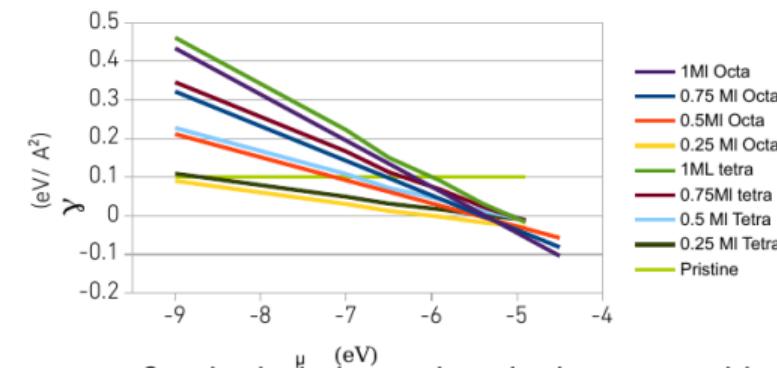
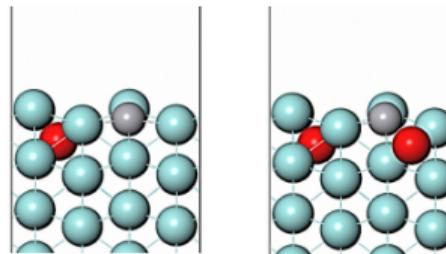
- Standard and Technical documentation interpretation.
- comparison of chemical analysis methods.
- Quality assurance related stuff:
  - documentation registries and archiving
  - documentation codification

# Zr(1010) 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

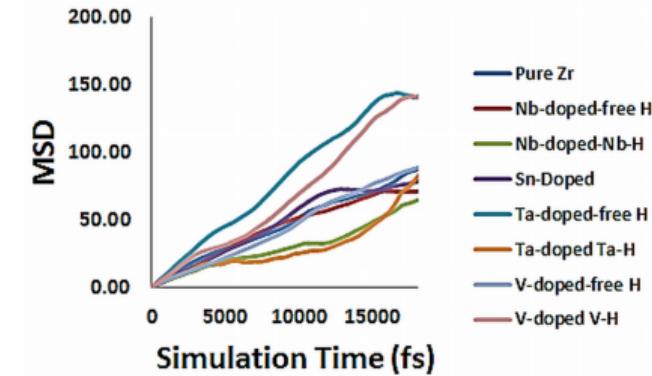
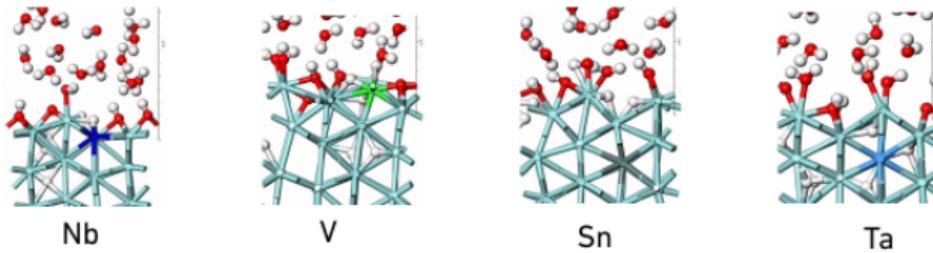


# Zr(1010) surface, Oxygen and Hydrogen Absorption

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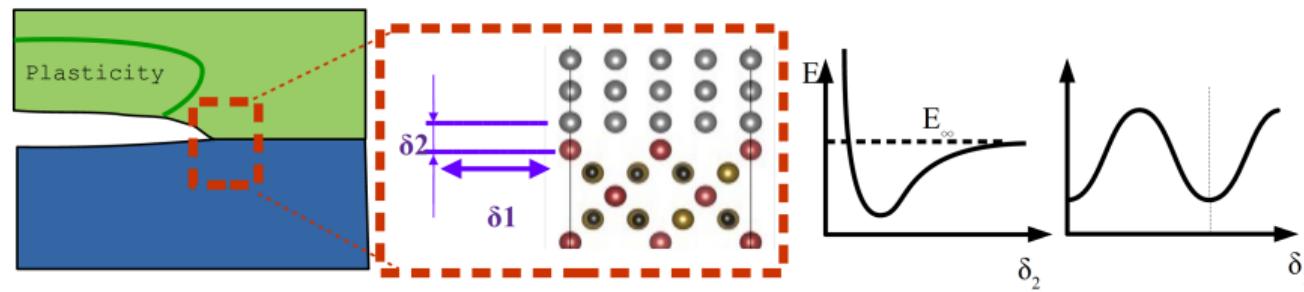
Progress so far

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

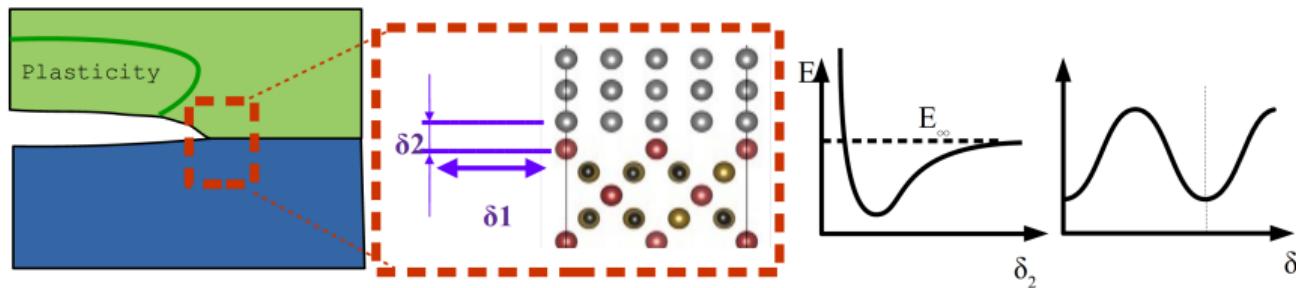


# Adhesion in FeBCC/Fe<sub>3</sub>O<sub>4</sub> interface

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!



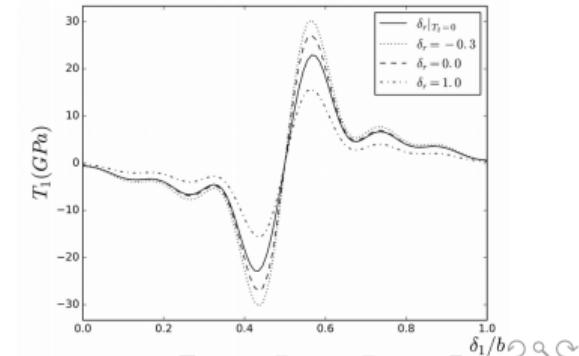
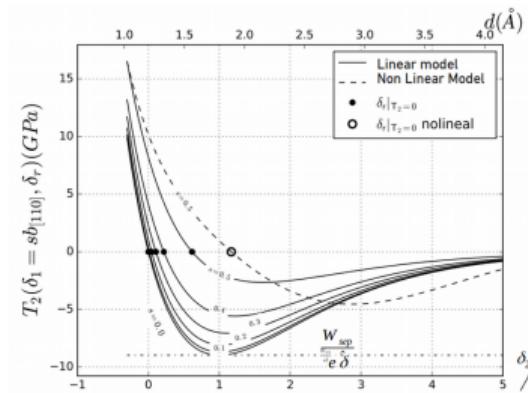
# Adhesion in FeBCC/Fe<sub>3</sub>O<sub>4</sub> interface



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

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

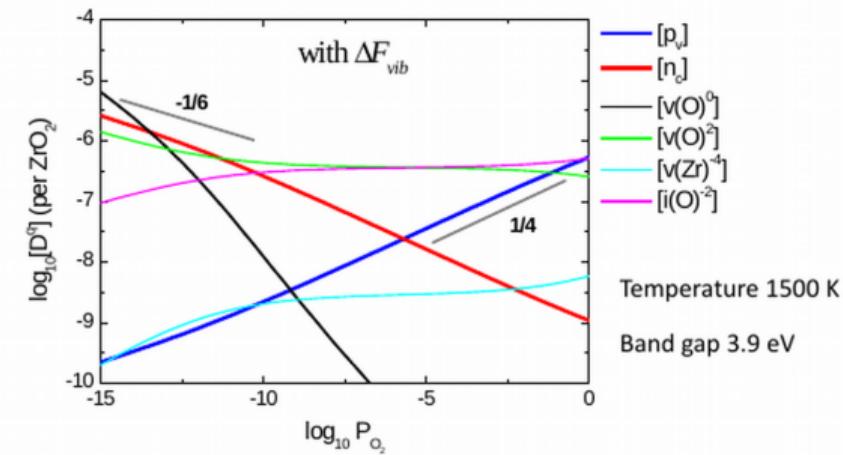
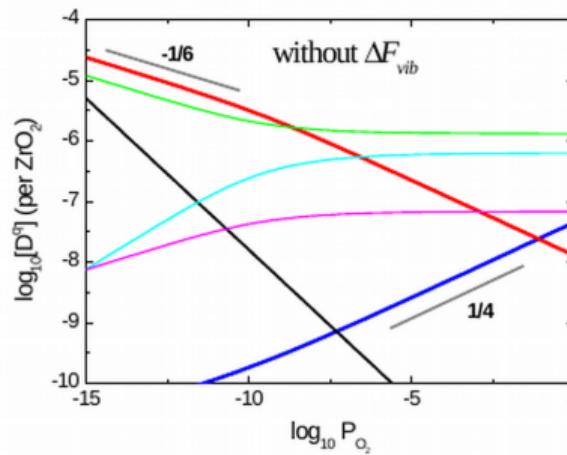
$$T_2(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_2}$$



# 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.

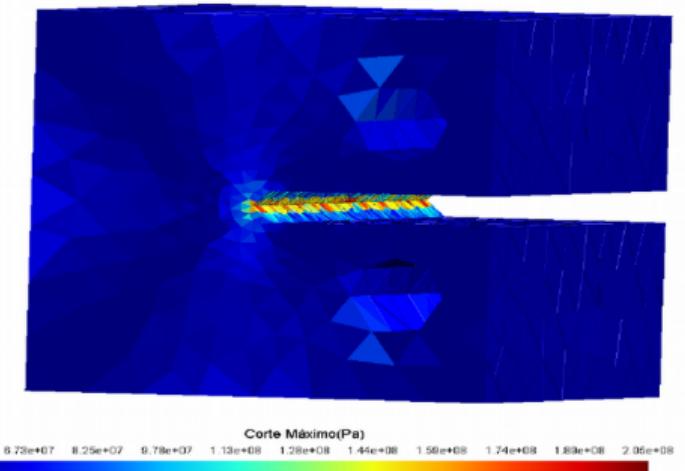
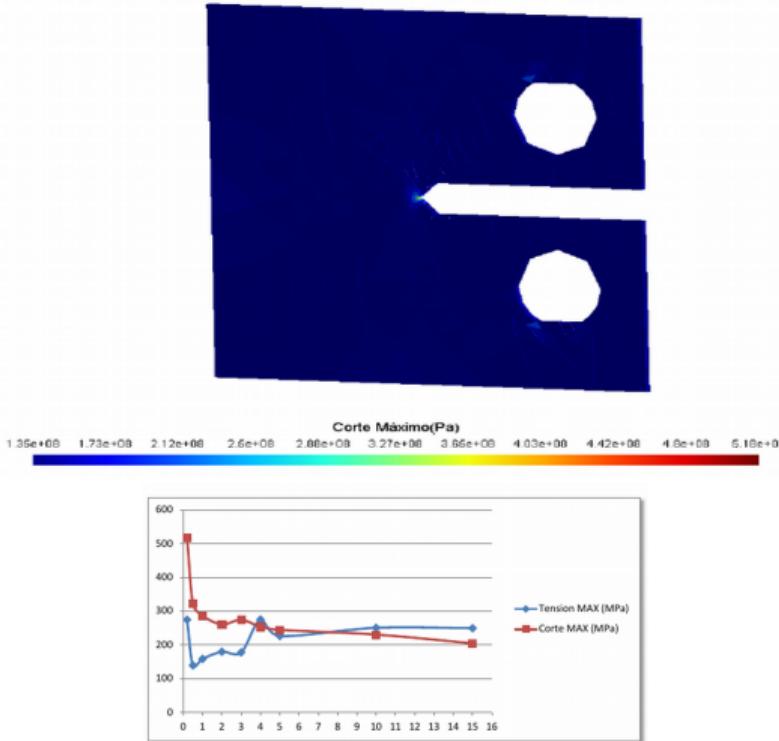
$$\Delta E_{D,q}^f = E_{\text{tot}}^{\text{DFT}}(D^q) - E_{\text{tot}}^{\text{DFT}}(\text{perfect}) - \Delta n_D \mu_D + q(E_{\text{VBM}} + \mu_F)$$



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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 16:59  /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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