

Density Functional Theory applied to interfaces, surfaces and oxides

Mariano Forti

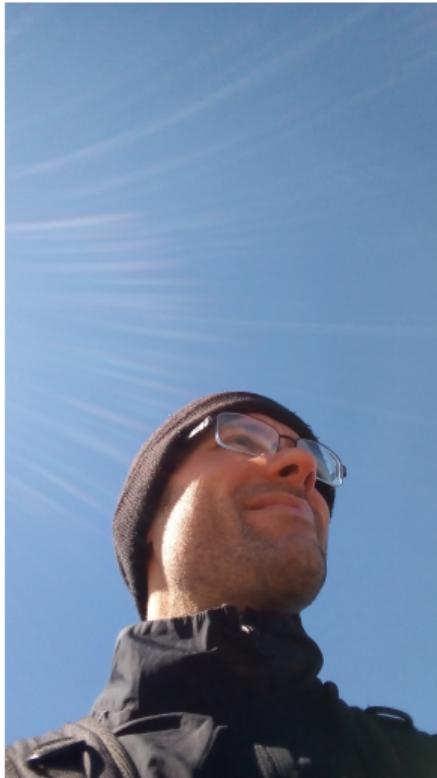
2019

and also an outline of other activities

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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.

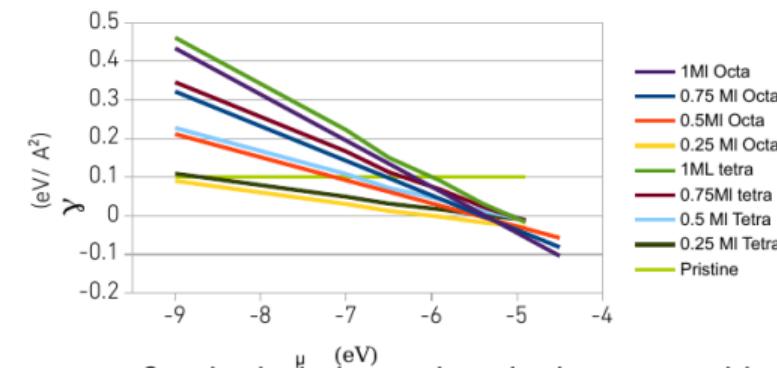
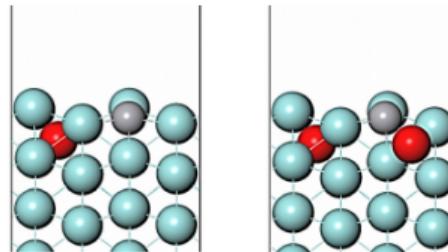
- Standard and Technical documentation interpretation.
- Comparison of chemical analysis methods.
- Quality assurance related stuff:
 - documentation registries and archiving
 - documentation codification

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

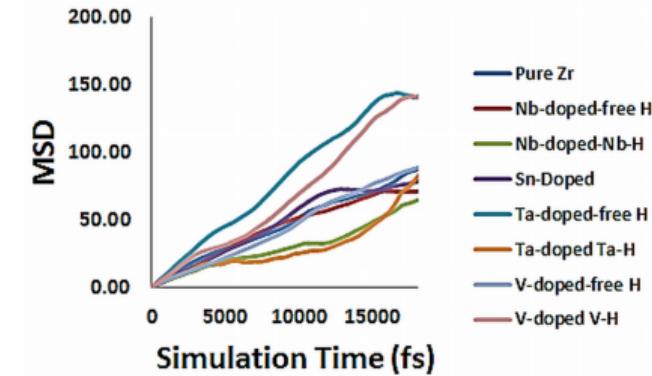
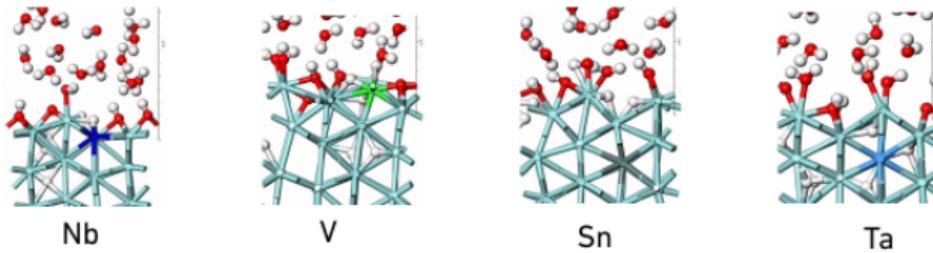


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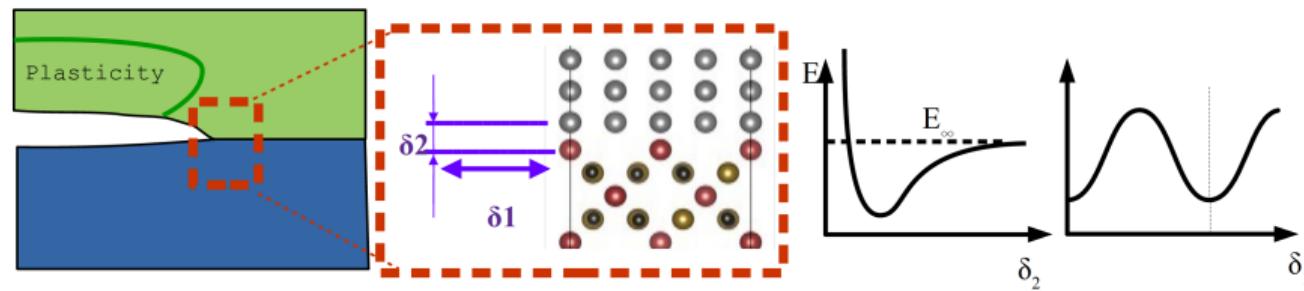
Progress so far

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

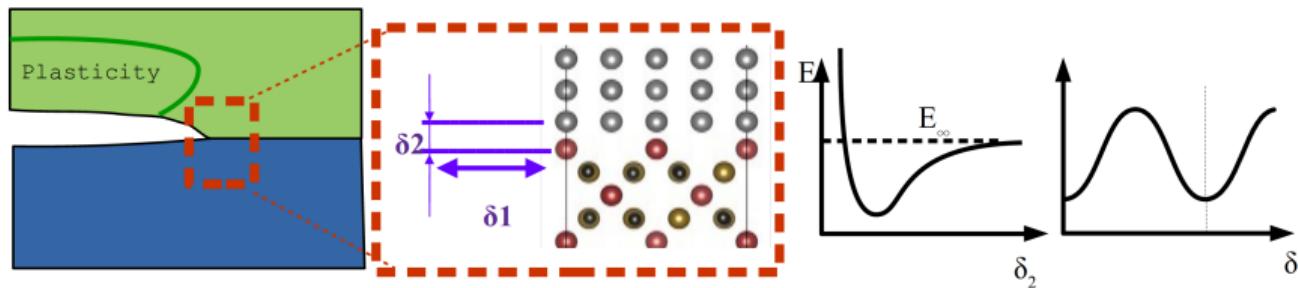


Adhesion in FeBCC/Fe₃O₄ interface

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!



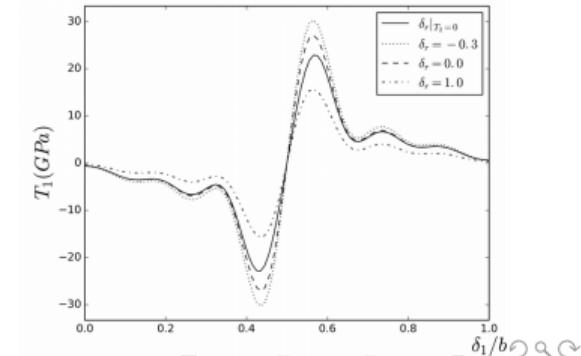
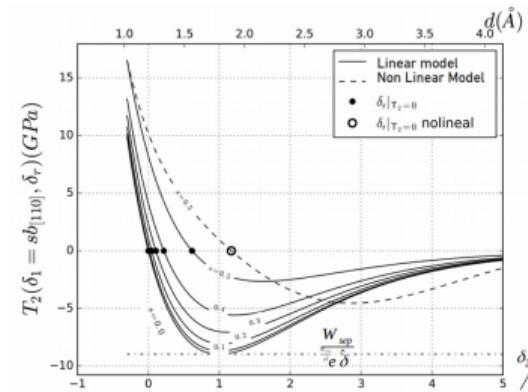
Adhesion in FeBCC/Fe₃O₄ interface



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

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

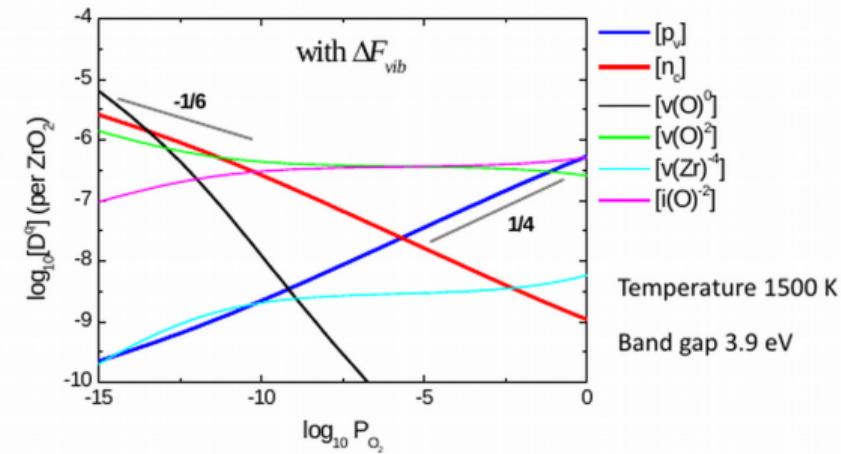
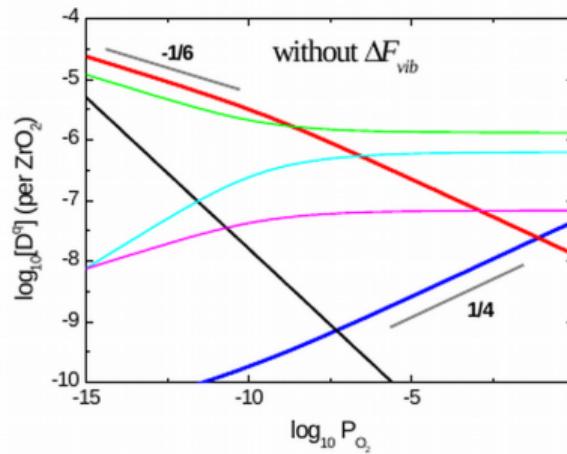
$$T_2(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_2}$$



Point Defect Equilibria in tetragonal ZrO₂

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.

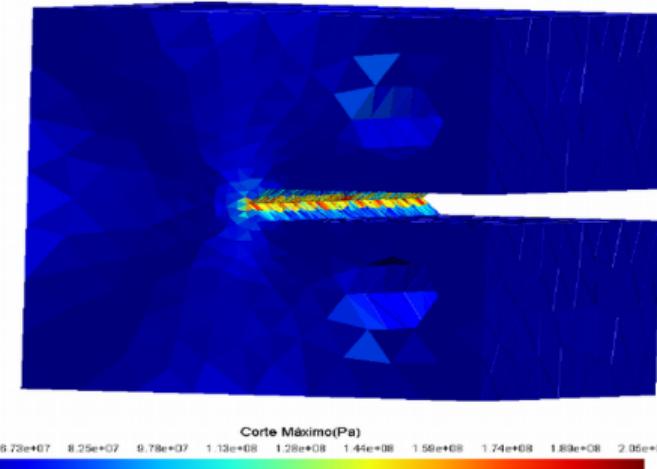
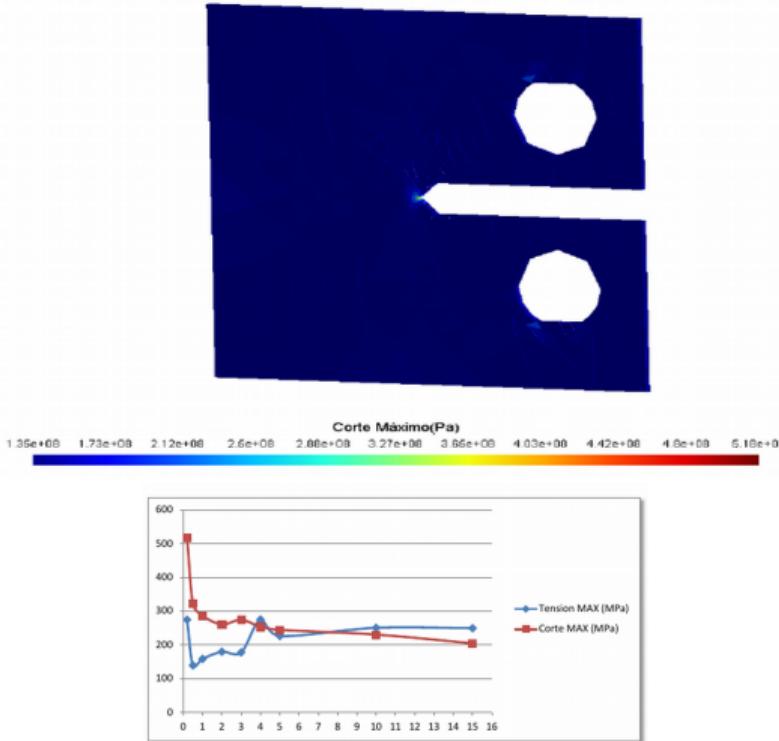
$$\Delta E_{D,q}^f = E_{\text{tot}}^{\text{DFT}}(D^q) - E_{\text{tot}}^{\text{DFT}}(\text{perfect}) - \Delta n_D \mu_D + q(E_{\text{VBM}} + \mu_F)$$



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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

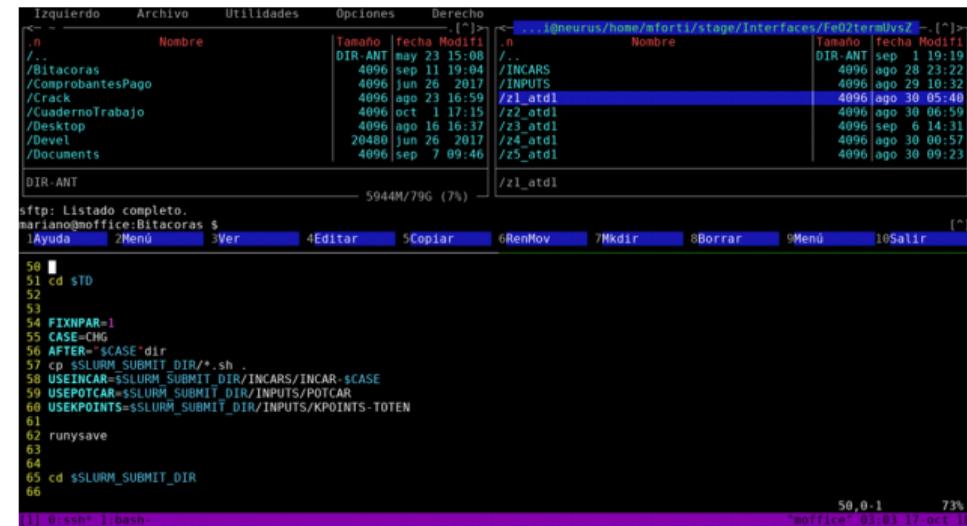
Workflow and Programming

■ Programming, Mainly scripting

- Mainly Bash,
- FORTRAN
- Python
- MATLAB®
- Couple Markup Languages (HTML, L^AT_EX , Markdown)

■ Worflow Solutions, allways evolving

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



The screenshot shows a terminal window with two panes. The left pane lists files in a directory structure, including sub-directories like /Bitácoras, /ComprobantesPago, /Crack, /CuadernoTrabajo, /Desktop, /Devel, and /Documents. The right pane shows a list of files in a sub-directory, with one file named 'z1_atdl' highlighted. Below the panes is a command-line interface with a menu bar at the top. The menu bar includes options like 'Menú', 'Ver', 'Editar', 'Copiar', 'RenMov', 'Mkdir', 'Borrar', 'Menú', and 'Salir'. The main area of the terminal shows a series of command-line entries, starting with 'sftp: Listado completo.' followed by several lines of file paths and file operations. At the bottom of the terminal window, there is status information including '50,0-1' and '73%', along with a timestamp '02:03 17-oct-18'.

```
sftp: Listado completo.
mariano@office:Bitácoras $ 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
[1] 0:ssh* 1:bash-
```

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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