

Density Functional Theory applied to Interface Adhesion, Surfaces and Oxides

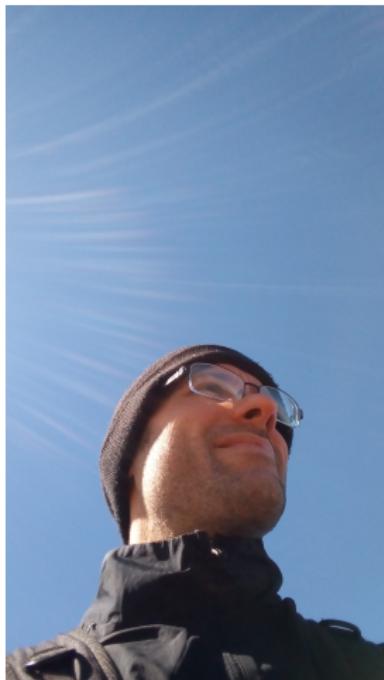
Mariano Forti

2019

An outline of my experience
Interview for a postdoctoral position at Helmholtz Centre Potsdam
Atomistic Modeling of (geo) Materials Professor Maribel Nuez
Valdez

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

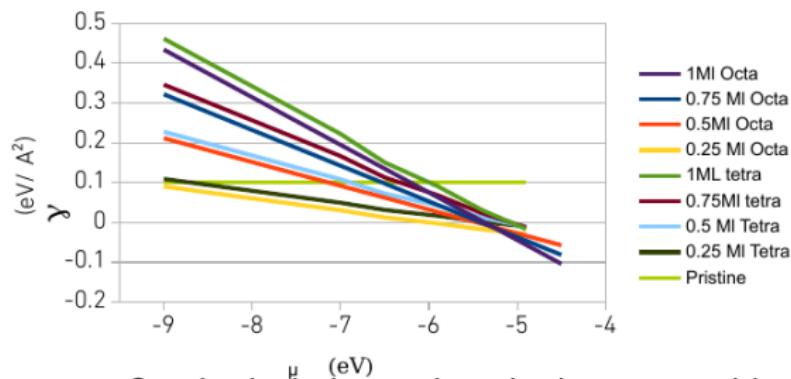
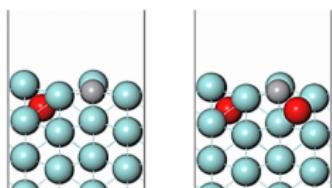
Current Research

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

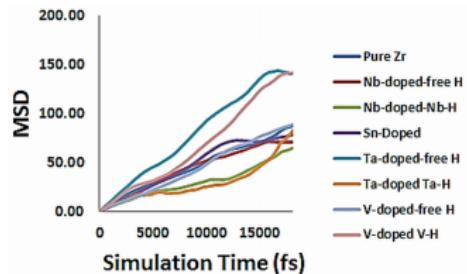
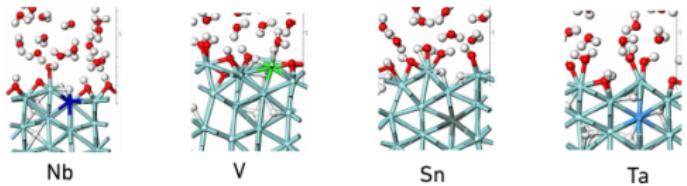


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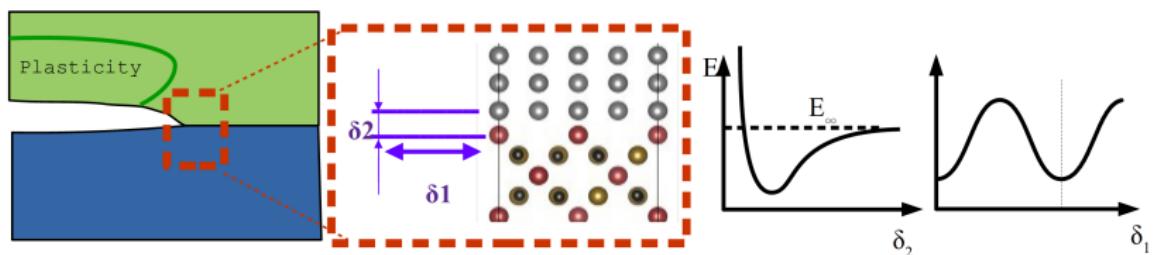
Progress so far

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

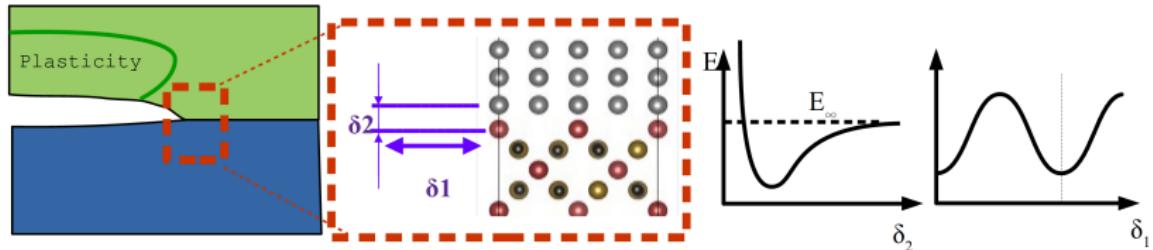


Adhesion in FeBCC/Fe₃O₄ interface

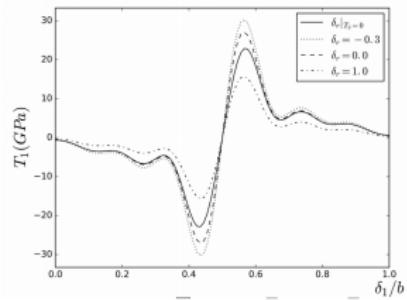
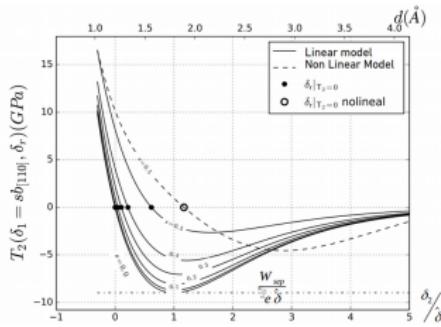
Separating the parts of the interface it is possible to obtain energy vs separation curves from DFT calculations. Then the forces can be obtained from interface potential models!



Adhesion in FeBCC/Fe₃O₄ interface



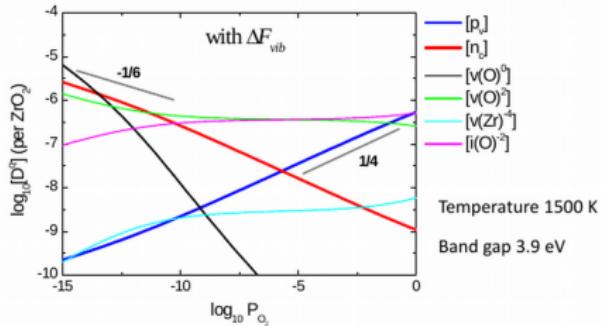
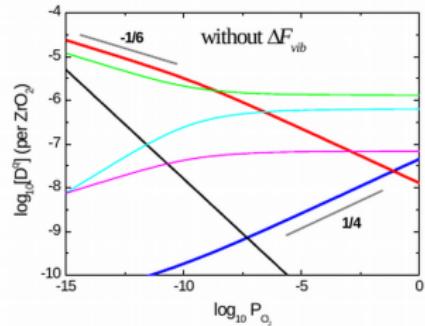
$$\tilde{L}_{\delta_1} = \frac{E_{\text{ad}}}{W_{\text{sep}}} = \exp\left(\frac{\delta_2}{\delta}\right) \sum_{i=0}^{i_{\max}} (1+\beta)^i \left[-1 + f(\delta_1)(1+\beta)^i \right] \alpha_i \left(\frac{\delta_2}{\delta} \right)^i \quad T_1(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_1} \quad T_2(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_2}$$



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.

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



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

Teaching

Teaching FEM basics

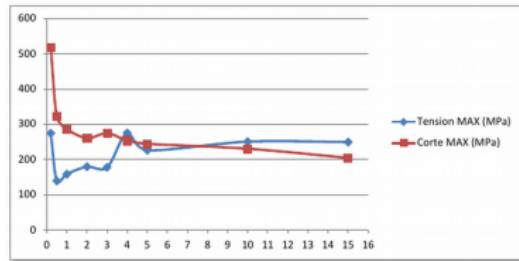
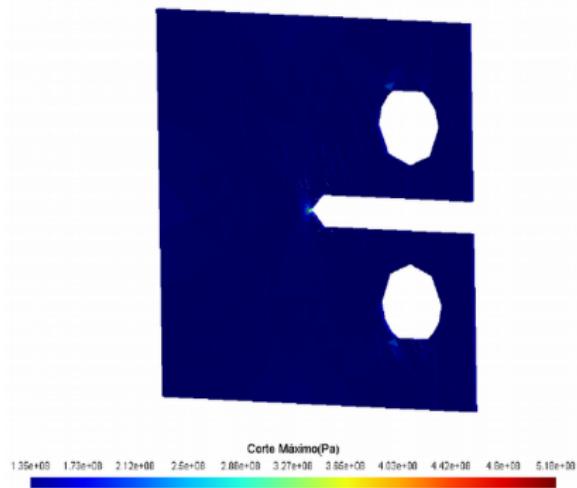
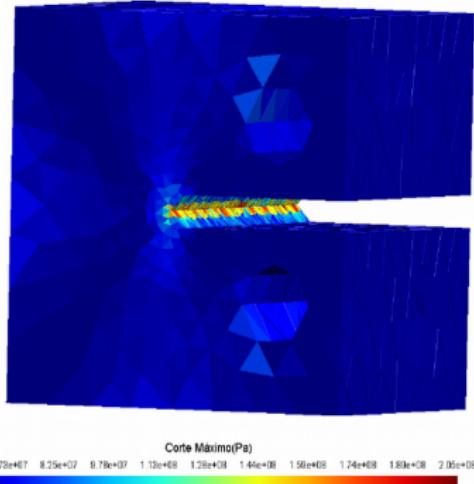


Fig. 11: Ordenadas: tensiones en MPa. Abscisas: espesor en cm.



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

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 image shows a composite screenshot of a Linux desktop environment. On the left, a terminal window displays a command-line session with several lines of code related to job submission and file management. In the center, a file browser window shows a directory tree with files and sub-directories. On the right, a status bar at the bottom of the screen displays system information such as battery level (50%, 0-1), signal strength, and other system metrics.

```
50 1
51 cd $TO
52
53
54 #EXHPAR>1
55 CASE<CHG
56 #SBATCH --ntasks=1 --gres=gpu:1
57 #SBATCH --mem=16G
58 #SBATCH --output=DIR/INCARS-%CASE%
59 #SBATCH --error=DIR/INPUTS/POTCAR
60 #SBATCH --cpus-per-task=1
61 #SBATCH --time=00:00:00
62 #SBATCH --qos=qosname
63
64 cd $SLURM_SUBMIT_DIR
65
66
```

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



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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