Density Functional Theory applied to interfaces, surfaces and oxides

Mariano Forti

2019

and also an outline of other activities

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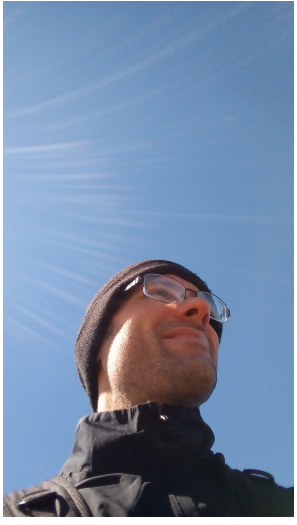
Who am I

Who am I?



Current positions

Comisión Nacional de Energía Atómica

División Aleaciones Especiales

INSTITUTO DE TECNOLOGÍA SABATO 25 Años

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

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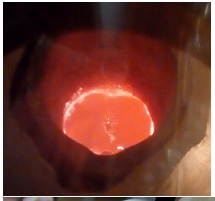
Current Research

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.

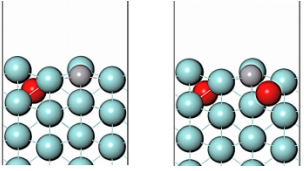
- Standard and Technical documentation interpretation.
- Comparison of chemical analysis methods.
- Quality assurance related stuff:
  - documentation registries and archiving
  - documentation codification

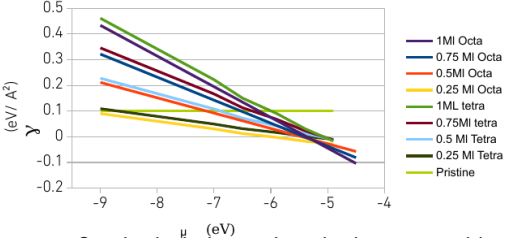
Zr(10$\bar{1}$0) surface, Oxygen and Hydrogen Absorption

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(10$\bar{1}$0) surface, Oxygen and Hydrogen Absorption

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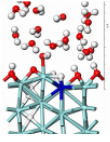
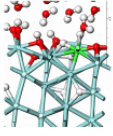
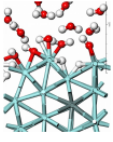
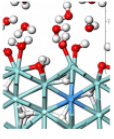
Progress so far

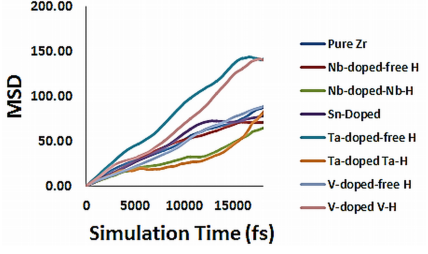
- Oxygen Coverage with alloy elements
- AIMD: Hydgrogen moves differently in the presence of Ta and V,


Nb


V

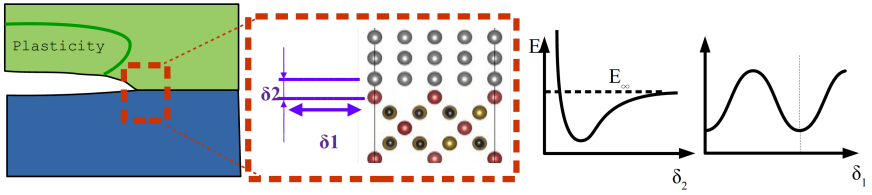

Sn


Ta

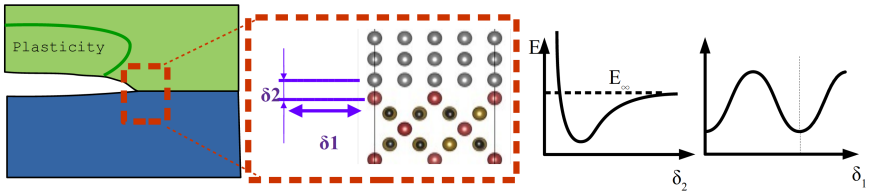


Adhesion in FeBCC/Fe_3O_4 interface

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!



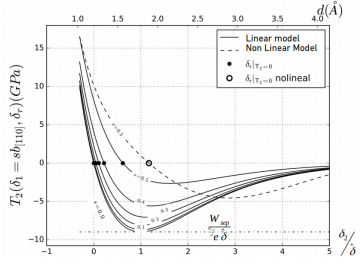
Adhesion in FeBCC/Fe_3O_4 interface

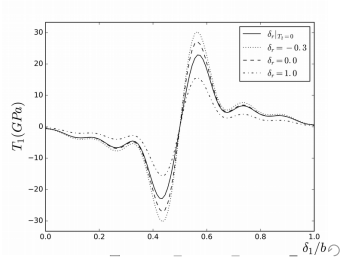


$$\tilde{L}_{\delta_1} = \frac{E_{ad}}{W_{sep}} = \exp\left(\frac{\delta_2}{\delta}\right) \sum_{i=0}^{i_{max}} (1+\beta)^i \left[-1 + f(\delta_1)(1+\beta)^i\right] \alpha_i \left(\frac{\delta_2}{\delta}\right)^i$$

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

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

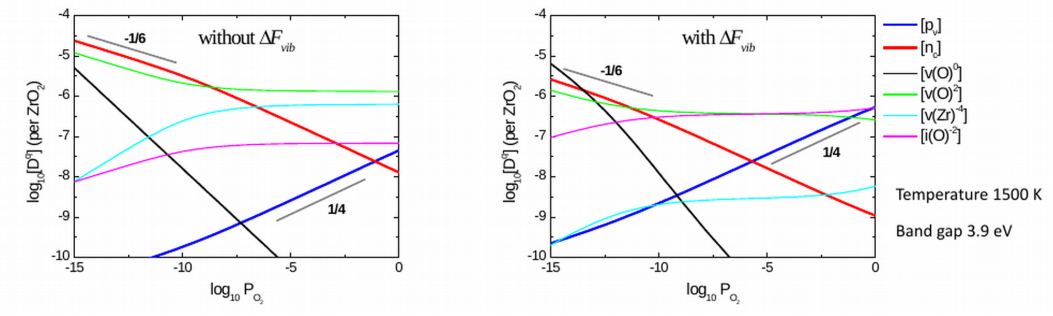




Point Defect Equilibria in tetragonal ZrO_2

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.

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



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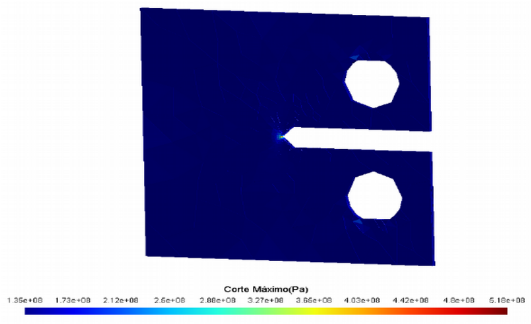
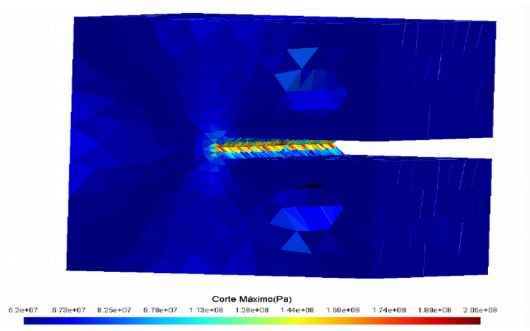
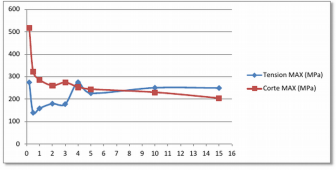
Teaching

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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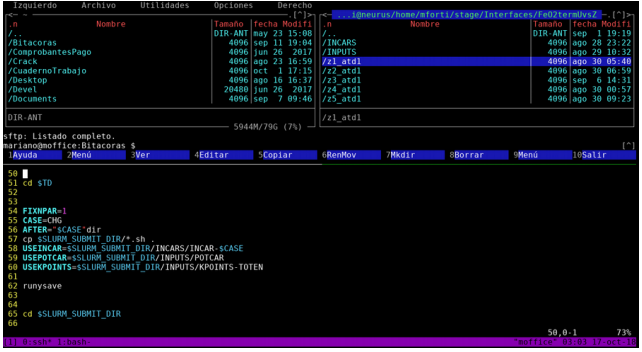
Other Skills

Workflow and Programming

- Programming, Mainly scripting
  - Mainly Bash,
  - FORTRAN
  - Python
  - MATLAB®
  - Couple Markup Languages (HTML, LaTeX , Markdown)
- Worflow Solutions, allways evolving
  - bash, tmux and vim
  - KDE
  - local git repositories for versioning and history
  - ssh, sftp
  - Libreoffice and MSOffice



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

Linux Sysadmin

- Installation and mantainance of small Rocks Clusters
- Compilation and mantainance 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 admininstration can give me a good insight in everyday work
- experience in interacting in multidisciplinary workgroups.

Any Questions?