EleonoraRomeo

contact

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in elero93

languages

Italian mother tongue
English medium-high

Computer skills

Crystal ●●●●○
Orca ●●○○○
Gaussian ●●○○○
Avogadro ●●●○○
Moldraw ●●●○○
DLV ●●●○○
Jmol ●●○○○
Ubuntu & Fedora ●●●●○
Windows ●●●●○
Office ●●●●○
Gimp ●●●○○
HTML ●●○○○

Experience

Oct 20 - Jan 21 **Department of Chemistry** — University of Turin
Recipient of scholarship
Computational study of vanadyl-anatase catalyst for the selective catalytic reduction of NOx

Oct 20 - Jan 21 **Department of Chemistry** — University of Turin
laboratory assistant
Teaching support in laboratory

21 - 25/09/20 **MSSC2020 school - Ab initio Modelling in Solid State Chemistry** — Imperial College London
Tutor

2012–2020 **Private lessons**
in chemistry, physics and mathematics for middle and high school students

2018–2020 **"Scuola dei Compiti" project** — Comune di Torino
Tutor
Chemistry and Mathematics tutor for high school students

2013–2017 **Department of Chemistry** — University of Turin
Students' representative

2013–2017 **Sports summer camp** — SiSport Fiat
Children's entertainer

2015–2018 **Giovani per Torino** — Torino
Volunteer

Education

2017–2020 **Master Degree** in Chemistry — University of Turin
Thesis title: "Computational study of surface catalysis on anatase"
Advisor: prof. Anna Maria Ferrari
Mark 110/110

Sep–Nov 19 **Erasmus Traineeship** — Imperial College London
Project title: "Studying bulk and surface properties of titanium dioxide"
Tutor: Giuseppe Mallia

Sep 19 and 20 **MSSC Crystal School** — Imperial College London

2012–2017 **Bachelor Degree** in Chemistry — University of Turin

2007–2012 **Scientific High School** — Turin

Research Themes

Master degree thesis: The study is focused on the structure of the catalyst vanadyl-anatase system involved in the Selective Catalytic Reduction (SCR) process, which demolishes the polluting NO_x, reducing it in N_2, in presence of NH_3. The attractiveness is modelling structure to show how the catalyst and the reducing agent interacts: this means examination of the anatase surface preferred, the vanadyl (VO^{2+}) coordination - octahedral on (001) anatase facet, tetrahedral on (101) - and the NH_3 inclinations to bind to Lewis (vanadium) or Brønsted acid site (V-OH), which seems to depend on both the surface and the coverage. All these valuation are done looking at the energies of static calculations. Since V reduce and re-oxidize during the process, Electronic Paramagnetic Resonance (EPR) parameters are calculated to prove the existence of V(IV) and complex which takes shape on the surface at this oxidation state.
Erasmus Traineeship project: Modelling anatase bulk, surface and slab. Also a furthered study of $VO(H_2O)_5$ complex is done, varying the basis set of vanadium, oxygen and hydrogen and the DFT functional; the aim was to practice with the Crystal program, with the notions learned during the computational chemistry course and to understand the electronic configuration of VO^{2+}.

Professional Skills

- Running calculation for geometry optimization, EPR parameters and simulating band structure and density of state (DOSS) with Crystal program
- Static calculations
- Modelling surface with cutting the slab and integrating adsorbed species
- Good knowledge of Gaussian and Orca
- Image manipulation with Avogadro, Jmol, DLV an Moldraw.

Licenses & Certifications

ECDL	**European Computer Driving Licence**
MIP	**Lifeguard licence for swimming pool, river, lake and sea**
CRI	**First Aid**

Soft Skills

Listening, Adaptability, Creativity, Desire to learn, Flexibility, Organization, Innovation, Logical thinking, Willingness to learn, Public speaking.

Interests

Professional	**-** To continue learning, work and to develop a career as researcher.
Personal	**-** Be economically independent; have a balance between my work and my personal life; manage my time in the activities that I like, such as music, cooking, gardening, reading (essay, fantasy and science fiction books), sport like swimming, skiing, trekking.