Francesca Menescardi

Info

Date of Birth: *17/02/1992*
Nationality: *Italian*

Email: francesca.menescardi@gmail.com
fmenesca@sissa.it

Work Experiences

2023- **Full-time Researcher**, Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, 34136, Trieste (TS)

2021- 2023 **Post-Doctoral Researcher in Geochemistry**, Università degli Studi di Genova, DISTAV department, Corso Europa, 26, 16132 Genova (GE)

Education

2017 -2021 **PhD in Chemistry**, Università degli Studi di Milano, Milan, Italy–Title obtained on 24/03/2021
Title: "*High-pressure materials discovery with advanced computational methods*"

2014-2016 **Master Degree in Chemical Sciences,** Università degli Studi di Milano, Milan, Italy, grade 110/110
Title: "*Electronic, optical and mechanical properties of π-conjugated carbon and silicon rings: a first-principles investigation*"

2011-2014 **Bachelor in Chemistry,** Università degli Studi di Milano, Milan, Italy
Title: "*Idrocarburi nel mezzo interstellare: studio first-principles dello ione CH_4^+ e dei suoi prodotti di dissociazione*"

Publications

- Menescardi, F., Ceresoli, D., & Belmonte, D. (2024). Melting Behavior of CaO at High Temperature and Pressure: A Molecular Dynamics Study. *The Journal of Physical Chemistry C*, *128*(43), 18498-18508. (DOI: 10.1021/acs.jpcc.4c04752)
- Ardit, M., Conte, S., Belmonte, D., Menescardi, F., Pollastri, S., Cruciani, G., & Dondi, M. (2023). Structure Evolution of Ge-Doped CaTiO3 (CTG) at High Pressure: Search for the First 2: 4 Locked-Tilt Perovskite by Synchrotron X-ray Diffraction and DFT Calculations. Inorganic Chemistry, 62(41), 16943-16953 (DOI: 10.1021/acs.inorgchem.3c02645)
- Ehrenreich-Petersen, E., Hansen, M. F., Jeanneau, J., Ceresoli, D., Menescardi, F., Ottesen, M., ... & Bremholm, M. (2023). Seven-Coordinated High-Pressure Phase of CrSb2 and Experimental Equation of State of M Sb2 (M= Cr, Fe, Ru, Os). Inorganic Chemistry, 62(31), 12203-12212. (DOI: 10.1021/acs.inorgchem.3c00227)
- Kronbo, C. H., Ehrenreich-Petersen, E., Ottesen, M., Menescardi, F., Ceresoli, D., & Bremholm, M. (2022). High-Pressure, High-Temperature Studies of Phase Transitions in SrOsO3— Discovery of a Post-Perovskite. *Inorganic Chemistry*. (DOI: 10.1021/acs.inorgchem.2c02471)
- Belmonte, D., La Fortezza, M., & Menescardi, F. (2022). Ab initio thermal expansion and thermoelastic properties of ringwoodite (γ-Mg 2 SiO 4) at mantle transition zone conditions. *European Journal of Mineralogy*, 34(2), 167-182. (DOI: 10.5194/ejm-34-167-2022)
- Menescardi, F, Ehrenreich-Petersen, E., Ceresoli, D. (2021). High pressure computational search of trivalent lanthanide di-nitrides. *The Journal of Physical Chemistry C*, 125, 161-167. (DOI: 10.1021/acs.jpcc.0c08904)
- Menescardi, F, Ceresoli, D. (2021). Comparative analysis of DFT+U, ACBNo, and Hybris Functionals on the Spin Density of $YTiO_3$ and $SrRuO_3$. *Applied Sciences*, 11, 616. (DOI: 10.3390/app11020616)
- Kronbo, C. H., Jensen, L. R., Menescardi, F., Ceresoli, D., & Bremholm, M. (2020). High-pressure, low-temperature studies of phase transitions in SrRuO3–Absence of volume collapse. *Journal of Solid State Chemistry*, 287, 121360. (DOI: 10.1016/j.jssc.2020.121360)
- Kronbo, C. H., Menescardi, F., Ceresoli, D., & Bremholm, M. (2021). High pressure structure studies of three SrGeO3 polymorphs–Amorphization under pressure. *Journal of Alloys and Compounds*, 855, 157419. (DOI: 10.1016/j.jallcom.2020.157419)

Teaching Experiences

5-6/2022 **Tutoring Activity,** course of Complementi di Matematica del CDS in Chimica, Università degli Studi di Milano, Dipartimento di Chimica (elena.zampieri@unimi.it)

5-6/2022 **Tutoring Activity,** course of Complementi di Matematica del CDS in Chimica Industriale, Università degli Studi di Milano, Dipartimento di Chimica (simone.scacchi@unimi.it)

10/2019 **Teaching Assistant,** course of Solid State Chemistry, Aarhus University, Chemistry Department (bremholm@chem.au.dk)

Oral Presentations and Posters

05/2024 "**A novel neural network potential to determine the melting temperature of crystals: the case study of CaO ",** poster presentation during Machine Learning Modalities for Materials Science workshop in Ljubljana

01/2023 "**Molecular dynamics strategies to determine the melting curve of CaO",** poster presentation during the 21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods in Trieste

09/2022 "**Molecular dynamics strategies to determine the melting curve of CaO",** flash talk during 4th Joint AIC-SILS Conference in Trieste

07/2022 "**Investigating thermodynamic properties of the deep Earth: a computational approach",** talk during 1° Congresso della Società Geochimica Italiana in Genova

08/2020 "**High pressure computational search of trivalent di-nitrides",** poster presentation during Quantum Crystallography Online Meeting

01/2019 **"Towards realistic DFT predictions of materials at high pressure",** poster presentation during the "Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials

11/2018 **"High pressure materials discovery with advanced DFT methods",** oral presentation during a CMC meeting in Goettingen, 8-10/11/2018

Prizes

09/2022 **Best Flash-Talk Presentation,** at the 4th Joint AIC-SILS Conference in Trieste

Formative Experiences

9-12/2019 **Three Months Staying in Denmark,** at Aarhus University, Chemistry Department, under the supervision of prof. Martin Bremholm (bremholm@chem.au.dk)

2009-2010 **Year Abroad as an Exchange Student,** ten months in Bow, NH, USA, where I attended the Senior Year in Bow High School

IT Competences

Application softwares Microsoft Office, Gaussian09, Quantum Espresso, USPEX, CRYSTAL17, LAMMPS
Graphic softwares Avogadro, Jmol, Molekel, XMGrace, GIMP, VESTA
Programming Python3, C++ (basis), Fortran90 (basis), Bash, LaTeX