



Elettra Sincrotrone Trieste

# Postdoctoral Research Associate for Theoretical Linear and Non-linear X-ray spectroscopy of chiral molecules in solution within the CHIRAX ERC grant

Deadline: 17 April 2025

Ref: DB/25/8

## Background

Elettra Sincrotrone Trieste is an international multidisciplinary research center operated as a user facility, featuring a 2.0/2.4 GeV, third-generation synchrotron light source (Elettra), a new free-electron laser light source (FERMI) and a variety of support laboratories. The extremely high quality of the machines and beamlines has set new performance records and has been producing results of great scientific and technological interest. In order to allow the laboratory to remain competitive in the next 20 years, an entirely new source - Elettra 2.0 - belonging to the new generation of storage rings (DLSR or Diffraction Limited Storage Ring) is being developed. The new source will exhibit a major increase in the brilliance and coherence fraction of the photon beams. The Elettra 2.0 optics is based on our enhanced symmetric six bend achromat structure (S6BA-E) with a 12-fold symmetry and an emittance of 200 pm-rad at 2.4 GeV. The new structure creates also straight sections in the arcs permitting the installation of additional insertion devices, thus increasing the number of beamlines. Existing beamlines will have to be upgraded and new beamlines developed to take full advantage of the characteristics of Elettra 2.0. The new machine is scheduled for commissioning in the second half of 2026. See <http://www.elettra.eu> for more information.

## Beamline/Activity/Project description

The CHIRAX project (<https://chirax.elettra.eu/>) funded by the European Research Council aims at implementing steady-state and time-resolved X-ray spectroscopy of chiral molecules in solution using circular and helical dichroism. The steady-state part is carried out at synchrotrons, while the time-resolved ones will exploit both synchrotrons and XFELs. The CHIRAX team has several strong national and international collaborations with theoreticians.

## Job description

The successful candidate will perform electronic structure calculations to predict chiral signals from X-ray absorption and chiral (circular and helical dichroism) spectroscopies, as well as nonlinear optical/X-ray methods of molecules in solution using *ab initio* quantum chemistry packages. Such chiral signals often involve multipoles of higher orders than the usual transition electric dipoles and their accurate computation is indispensable. The successful candidate is expected to foster ongoing collaborations of the CHIRAX team with theoreticians and develop new ones. Elettra Sincrotrone Trieste possesses computational facilities, but access to larger external facilities is also foreseen. Specifically, the successful candidate is expected to apply for computation time at national and international computational facilities such as CINECA and the Molecular Foundry. Analysis of results, writing-up of reports and papers, presentation at conferences and workshops is expected.

## Qualifications

A PhD in Physics, Physical Chemistry, Computational Chemistry or related discipline with specific expertise in quantum chemistry, theoretical spectroscopy and theory of non-linear phenomena is required. The candidate should have earned his/her PhD no more than 6 years ago.

Applications will be considered also from candidates who have completed their doctoral research, but for whom the defense is scheduled to take place.

The following qualifications will be considered as positive assets:

- Experience in the theory of X-ray spectra and/or molecular systems
- Experience in simulations of XFEL and/or synchrotron results

### Elettra - Sincrotrone Trieste S.C.p.A.

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The successful candidates should possess strong personal skills favouring collaborative research programs in a team-oriented environment.

Good time management skills and ability to prioritize are expected, together with the ability to interact with the facility staff and international users at all levels and to work as part of a multi-disciplinary team.

Good oral and written communication skills in English are essential.

## General information

The appointment will be a fixed term contract with an initial duration of 12 months, renewable upon agreement by the parties.

The salary will be commensurate with previous experience and qualifications of the candidate.

Applications should include a full curriculum vitae, the names and contact information (including electronic mail) of up to three persons who have agreed to provide references.

The interviews may be held via video conferencing.

The ranking of eligible candidates resulting from this selection procedure may be used for additional appointments within the following 24 months.

Employees or former employees of Elettra Sincrotrone Trieste S.C.p.A. or temporary and staff leasing employees or former employees with working experience at the company will be excluded from the present selection procedure. Employees or former employees of any Italian Public Entity who have exercised authority over Elettra Sincrotrone Trieste S.C.p.A. or have negotiated with Elettra - Sincrotrone Trieste S.C.p.A. within the last three years, will also be excluded from the present selection procedure, in accordance with the provisions of article 21 of the Italian legislative decree no. 39/2013 and in conjunction with article 53 (subsection 16ter) of Italian legislative decree no. 165/2001.

The deadline for the submission of the application is April 17, 2025.

**For further information please contact Prof. Majed Chergui: [majed.chergui@elettra.eu](mailto:majed.chergui@elettra.eu) ; [majed.chergui@epfl.ch](mailto:majed.chergui@epfl.ch)**

We thank all applicants in advance.

To apply for this position please visit the following link:

<https://www.elettra.trieste.it/it/about/careers/working-withus.html?id=4246>

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