NODOKA HARA

Ph.D. student
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SUMMARY

3rd year PhD student working on matter under extreme conditions (mainly high/extreme temperature) using advanced spectroscopic techniques, e.g. investigations of the local structure of matter at high temperatures with XAFS using both peak fitting and the RMC method. Currently, in collaboration with EuXFEL, we are developing a reconstruction code to deconvolve an inelastic X-ray scattering spectrum using the self-amplified spontaneous emission (SASE) pulse, the pink beam.

EDUCATION

Ph.D. of physics Dec 2021 - present
University of Camerino Camerino, Italy
Reconstruction of x-ray scattering spectra using the full SASE spectrum and local structure investigation with XAFS under the supervision of Prof. A. Di Cicco at Univ. Camerino in Italy and Dr. S. Pascarelli and Dr. U. Zastrau at EuXFEL in Germany

Master of Science, physics Apr 2020 - Sep 2021
University of Toyama Toyama, Japan
Thesis "Interpretation of Cohen-Fano effect in the framework of Multiple Scattering theory" supervised by Prof. K. Hatada at Univ. Toyama in Japan and Dr. Calogero R. Natoli at INFN-LNF in Italy

Bachelor of Science, physics Apr 2016 - Mar 2020
University of Toyama Toyama, Japan
Thesis "Implementation of the electric quadrupole transition term in FPMS code" supervised by Prof. K. Hatada at Univ. Toyama in Japan

PROJECTS

Ph.D.

- Working on a code development using an inverse matrix approach to deconvolve overlapped inelastic x-ray scattering (IXS) spectra due to a broadened energy width of the SASE pulse under the supervision of Prof. A. Di Cicco, Dr. S. Pascarelli and Dr. U. Zastrau. This approach would achieve high-resolved IXS measurement without seeding or monochromator using SASE spectra. Moreover, numerous photons in SASE are able to heat electrons to the warm dense matter (WDM) or the high energy density (HED) regime, so this method opens the possibility of discovering new physical phenomena under extreme conditions, such as the science of planetary interiors and inertial confinement fusion studies.
- Local structure investigation of solid and liquid Au by XAFS.
  The investigation of the local structure of Au as a function of temperature from 80-1400 K in solid and liquid phases by GnXAS code using L_1-, L_2-, and L_3-edge XAFS data simultaneously have been carried out , under supervision of Prof. A. Di Cicco. In addition, the application of the Reverse Monte Carlo (RMC) method has allowed us to obtain the three-dimensional structure.
- XAFS analysis code development to measure XAFS with SASE pulse at HED beamline, EuXFEL in collaboration with HED group at EuXFEL, Germany and Prof. Marion Harmand at IMPMC-CNRS, Sorbonne Université France.
- Local structure analysis of GeS_2, $GeSe_2$ and NiPd (Pd speciation in Ni-based industrial waste) with XAFS

Master and Bachelor

- Thesis work of Master "Interpretation of Cohen-Fano effect in the framework of Multiple Scattering theory"
  Investigated the interference between two atoms that occurred in XAFS the so-called Cohen-Fano effect mainly supervised by Dr. Calogero R. Natoli. Rewroted a better approximation for the effect and we have implemented it for absorption and photoemission spectroscopies in FPMS(Full Potential Multiple Scattering) program, which was originally developed by Prof. K. Hatada, then calculated for molecule N_2 in gas phase using this code.
- Relativistic effect in EXAFS using GnXAS.
  Investigated the relativistic effect for Br_2, $SiCl_4$, Ge, and crystalline Pb in EXAFS using GnXAS supervised by Prof. A. Di Cicco who developed GnXAS software and Dr. C. R. Natoli who implemented relativistic correction in it.
- Thesis work of Bachelor "Implementation of electric quadrupole transition term in FPMS code"
  Derived the formula of quadrupole transition within full potential multiple scattering theory and have implemented it in FPMS, then applied it to anatase and rutile TiO_2 XANES calculations under the supervision of Prof. K. Hatada.

PUBLICATIONS

- **Nodoka Hara**, Fabio Iesari, Toshihiro Okajima and Andrea Di Cicco, "Local structure of solid and liquid gold probed by Reverse Monte Carlo analysis of x-ray absorption data", *Journal of Synchrotron Radiation* (Accepted)
- Rodrigues, João E. F. S., Emin Mijit, Angelika D. Rosa, Laura Silenzi, **Nodoka Hara**, Catalin Popescu, José A. Alonso, Tetsuo Irifune, Zhiwei Hu, and Andrea Di Cicco, "Exploring the Interplay between Structure and Electronic Behavior across Pressure-Induced Isostructural and Structural Transitions in Weyl-Type Semimetal NbAs", *Crystals* **14**, 578 (2024)
- **Nodoka Hara**, Georghii Tchoudinov, Adriano Filipponi and Andrea Di Cicco, "Local structure of solid and liquid Au as a function of temperature by x-ray absorption spectroscopy", *Physical Review B* **107**, 184107 (2023)
- **Nodoka Hara**, Keisuke Hatada, and Calogero R. Natoli, "Multiple scattering description of multicenter coherent emission with applications to photoionization and electron scattering in diatomic molecules", *Physical Review A* **106**, 052807 (2022)
- G. Kastirke et. al., "Investigating charge-up and fragmentation dynamics of oxygen molecules after interaction with strong X-ray free-electron laser pulses", *Phys. Chem. Chem. Phys.*, **24**, 27121-27127 (2022).
- **Nodoka Hara**, Andrea Di Cicco, Georghii Tchoudinov, Keisuke Hatada, and Calogero R. Natoli, "Relativistic Corrections to Phase Shift Calculation in the GNXAS Package", *Symmetry* **13**, 1021 (2021).

SCHOLARSHIPS, GRANTS AND AWARDS

- **Full scholarship for the Ph.D. Program** — Dec 2021-Dec2024
  University of Camerino — Camerino, Italy
- **SILS 2024 conference grant** — Sep 2024
  SILS 2024, University of Calabria — Rende, Italy
- **SILS conference 2023 Poster award** — Sep 2023
  SILS 2023, University of Sapienza — Rome, Italy
  "Multiple scattering description of multicentre coherent emission in photoionization: the Cohen-Fano interference term in diatomic molecules revisited"
- **SILS 2023 conference grant** — Sep 2023
  SILS 2023, University of Sapienza — Rome, Italy
- **Erasmus + Traineeship** — Aug 2023
  University of Camerino — Camerino, Italy
- **Ultrafast X-ray Summer School 2023 grant** — June 2023
  UXSS 2023, DESY — Hamburg, Germany

- **Student award** Sep 2021
  24th Japan XAFS annual meeting Chiba, Japan (Online)
  "Relativistic corrections to phase shift calculation in the GNXAS package"

ORAL AND POSTER PRESENTATIONS

- N. Hara, U. Zastrau et. al., "Reconstruction of high-resolution inelastic X-ray scattering spectra collected by SASE XFEL" at SILS 2024 in Rende, Italy on 5 - 7 Sep 2024 (**Invited talk**)
- N. Hara, F. Iesari, T. Okajima and A. Di Cicco, "Local structure of solid and liquid gold probed by Reverse Monte Carlo analysis of x-ray absorption data" at SILS 2024 in Rende, Italy on 5 - 7 Sep 2024 (Oral)
- N. Hara, Georghii Tchoudinov, Adriano Filipponi and Andrea Di Cicco, "Local structure of solid and liquid Au as a function of temperature by XAFS" at SILS 2023 in Rome, Italy on 30 Aug - 1 Sep 2023 (Oral)
- N. Hara, A. Trapananti, U. Zastrau, O. S. Humphries, C. Milne, S. Pascarelli, K. Hatada and A. Di Cicco, "Investigation of the spectra reconstruction requirements of high-resolution inelastic X-ray scattering spectra using SASE radiation" at SILS 2023 in Rome, Italy on 30 Aug -1 Sep 2023 (Poster)
- Nodoka Hara, Keisuke Hatada, and Calogero R. Natoli "Multiple scattering description of multicenter coherent emission in photoionization: the Cohen-Fano interference term in diatomic molecules revisited" at SILS 2023 in Rome, Italy on 30 Aug -1 Sep 2023 (Poster) **Poster prize**
- N. Hara, A. Trapananti, U. Zastrau, O. S. Humphries, C. Milne, S. Pascarelli, K. Hatada and A. Di Cicco, "Investigation of the spectra reconstruction requirements of high-resolution inelastic X-ray scattering spectra using SASE radiation" at Students' and Science Days in Hamburg, Germany on 15-17 May 2023 (Poster)
- N. Hara, G. Tchoudinov, C. R. Natoli, A. Filipponi, and A. Di Cicco, "Relativistic effects in EXAFS: overview and application to gold" at the 4th Joint AIC-SILS Conference in Trieste, Italy on 12-15 Sep 2022 (Oral)
- N. Hara, G. Tchoudinov, C. R. Natoli, A. Filipponi, and A. Di Cicco, "Relativistic effects in EXAFS: overview and application to gold" at the 18th International conference XAFS 2022 (online) in Sydney, Australia on 10-15 Jul 2022 (Oral)
- N. Hara, A. Di Cicco, G. Tchoudinov, K. Hatada and C. R. Natoli, "Relativistic corrections to phase shift calculation in the GNXAS package" at the 24th Japan XAFS annual meeting (online) in Chiba, Japan on 1-3 Sep 2021 (Oral) **Student prize**
- N. Hara, A. Di Cicco, G. Tchoudinov, K. Hatada and C. R. Natoli, "Relativistic corrections to phase shift calculation in the GNXAS package" at the 17th International conference XAFS 2021 (online) in Sydney, Australia on 11-13 Jul 2021 (Oral)
- N. Hara and K. Hatada, "XANES calculation with Full Potential Multiple Scattering Theory considering electric quadrupole transition" at the 23rd Japan XAFS annual meeting (online) in Hiroshima, Japan on 9-11 Sep 2020 (Oral)
- N. Hara and K. Hatada, "Implementing electric quadrupole transition in FPMS" at Frontier of theoretical approaches in x-ray spectroscopies in Tukuba, Japan on 3-4 Oct 2019 (Poster)