# ASEEM R. KSHIRSAGAR


**Physicist | Computational Material Scientist**

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Rennes, France
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## EDUCATION

PhD in "*Ab initio* study of the excited state properties of photoresponsive metal-organic frameworks"

**SIMAP laboratory, University of Grenoble-Alps**

Nov 2017-Mar 2021 — Grenoble, France

Bachelor of Science-Master of Science (BS-MS) dual degree

**Indian Institute of Science Education and Research (IISER)**

Aug 2012- May 2017 — Pune, India

## RESEARCH EXPERIENCE

### MOPGA Fellow : Make Our Planet Great Again fellowship, Campus France and MEAE

*"Stabilizing halide perovskites for efficient and durable solar cells"*

**Rennes Institute of Chemical Sciences, CNRS, University of Rennes**

1 Dec. 2025 - Ongoing — Rennes, France

- Computation and analyses of NMR footprint of local structure in halide perovskite
- Theoretical investigation of photostability of halide perovskites

**Advisor**: Claudine Katan **Collaborators**: Jacky Even, Aditya Mohite

### Postdoctoral Fellow : Brittany Regional Fellowship for Sustainability Research

*"Optical properties of chiral metal-halide perovskites"*

**Rennes Institute of Chemical Sciences, CNRS, University of Rennes**

1 Dec. 2024 - Ongoing — Rennes, France

- Accurate computational description of circular dichroism in crystalline materials and identification of relevant structure-property relationship
- Theoretical description of lattice dynamics in 1D metal halides
- Side project: literature review on exciton-polarons in polar semiconductors

**Advisor**: Claudine Katan **Collaborators**: Mikaël Kepenekian, Jacky Even

### Postdoctoral Researcher

*"Resonant Raman scattering in $BiFeO_3$"*

**Department of Physics and Material Science, University of Luxembourg**

1 July 2021 - 30 Nov. 2024 — Luxembourg

- Study of spin-flip electronic excitations in $BiFeO_3$ using Bethe-Salpeter formalism and their possible use for light-induced spin-magnetization
- Tracing in-gap Raman resonance in $BiFeO_3$ to strong coupling of spin-flip electronic excitations with lattice vibrations
- Side projects: Raman scattering in $BaZrS_3$ and $BaHfS_3$, Ambipolar current-voltage behaviour of Ti-$WSe_2$ system

**Advisor**: Sven Reichardt **Collaborators**: Ludger Wirtz, Mäel Guennou, Georgy Gordeev

### Doctoral Researcher

*"Ab initio study of the excited state properties of azobenzene-functionalized photoresponsive metal-organic frameworks"*

**SIMAP laboratory (UMR5266), CNRS**

1 Oct. 2017– 31 Dec. 2020 Grenoble, France

- Unraveling microscopic mechanism of light-tunable $CO_2$ adsorption in photoresponsive metal-organic frameworks (MOFs), relevant for energy efficient $CO_2$ capture, using atomistic modeling
- Study of strongly bound electron-hole states in metal-organic frameworks (MOFs) and their implications on the optoelectronic potential of MOFs
- Proposing an efficient and accurate *ab initio* QM/MM method for computing optical excitation energies of solvated azobenzene-based photo-switches within GW-BSE formalism
- Side-project: Atomistic modeling of structural evolution of Pt nanoparticle in presence of CO gas
- Mentoring students of Grenoble-INP for semester project in the field of materials modelling

**Advisor**: Roberta Poloni **Collaborators**: Xavier Blase, Li-Chiang Lin, Claudio Attaccalite, Jing Li

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**MS thesis researcher**

*"First-principles investigation of 2D $MoS_2$-MXene heterostructures as cathodes in Mg-ion batteries"*

**Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)**

1 Apr. 2016 - 31 Mar. 2017 Bengaluru, India

- Proposing and modeling $MoS_2$-MXene heterostructure as a Mg-ion battery cathode to exploit both the fast diffusion channels offered by $MoS_2$ and large gravimetric capacity offered by MXenes

**Supervisor**: Umesh Waghmare **Co-supervisor**: Prasentjit Ghosh

# PUBLICATIONS

- Even, J., Thebaud, S., **Kshirsagar**, A. R., Pedesseau, L., Zacharias, M. & Katan, C. "Empirical approaches to Frohlich excitonic polarons in polar semiconductors with application to 3D halide perovskites". *arXiv* **2505.07406,** [cond-mat.mtrl–sci] (2025).
- **Kshirsagar**, A. R. & Reichardt, S. "Flipping of electronic spins in $BiFeO_3$ via chiral $d-d$ excitations". *Physical Review B* **112,** L121111 (12 Sept. 2025).
- Maniadi, M., Guesdon, M., Tieriekhov, K., **Kshirsagar**, A. R., Spirito, D., Martín-García, B., Mercier, N., Arteaga, O., Kepenekian, M., Katan, C. & Abhervé, A. "On the origin of circularly polarized luminescence in chiral one-dimensional (A)PbBr3 single crystals". *ChemRxiv (submitted of Chemistry of Materials, ACS)* (Dec. 2025).
- **Kshirsagar**, A. R. & Reichardt, S. "Understanding electronic excited states in $BiFeO_3$ via ab initio calculations and symmetry analysis". *Physical Review B* **110,** 155131 (2024).
- Yetkin, H. A., Dale, P. J., **Kshirsagar**, A. R., Reichardt, S., Latini, A., Ciccioli, A. & Romagnoli, L. "A Combined Theoretical and Experimental Raman Scattering Study of BaZrS3-BaHfS3 Solid Solutions". *ChemPhysChem* **25,** e202400340 (2024).
- **Kshirsagar**, A. R. & Poloni, R. "Assessing the Role of the Kohn-Sham Density in the Calculation of the Low-Lying Bethe-Salpeter Excitation Energies". *The Journal of Physical Chemistry A* **127,** 2618–2627 (2023).
- Ram, A., Maity, K., Marchand, C., Mahmoudi, A., **Kshirsagar**, A. R., Soliman, M., Taniguchi, T., Watanabe, K., Doudin, B., Ouerghi, A., Reichardt, S., O'Connor, I. & Dayen, J.-F. "Reconfigurable Multifunctional van der Waals Ferroelectric Devices and Logic Circuits". *ACS Nano* **17,** 21865–21877 (2023).
- Carnis, J., **Kshirsagar**, A. R., Wu, L., Dupraz, M., Labat, S., Texier, M., Favre, L., Gao, L., Oropeza, F. E., Gazit, N., Almog, E., Campos, A., Micha, J.-S., Hensen, E. J. M., Leake, S. J., Schülli, T. U., Rabkin, E., Thomas, O., Poloni, R., Hofmann, J. P. & Richard, M.-I. "Twin boundary migration in an individual platinum nanocrystal during catalytic CO oxidation". *Nature Communications* **12** (2021).
- **Kshirsagar**, A. R. *Ab initio study of the excited state properties of azobenzene-functionalized photoresponsive MOFs.* PhD thesis (Université Grenoble Alpes, 2021).
- **Kshirsagar**, A. R., Attaccalite, C., Blase, X., Li, J. & Poloni, R. "Bethe–Salpeter Study of the Optical Absorption of trans and cis Azobenzene-Functionalized Metal–Organic Frameworks Using Molecular and Periodic Models". *The Journal of Physical Chemistry C* **125,** 7401–7412 (2021).

- **Kshirsagar**, A. R., Blase, X., Attaccalite, C. & Poloni, R. "Strongly Bound Excitons in Metal–Organic Framework MOF-5: A Many-Body Perturbation Theory Study". *The Journal of Physical Chemistry Letters* **12,** 4045–4051 (2021).
- **Kshirsagar**, A. R., D'Avino, G., Blase, X., Li, J. & Poloni, R. "Accurate Prediction of the $S_1$ Excitation Energy in Solvated Azobenzene Derivatives via Embedded Orbital-Tuned Bethe-Salpeter Calculations". *Journal of Chemical Theory and Computation* **16,** 2021–2027 (2020).
- Yang, C.-T., **Kshirsagar**, A. R., Eddin, A. C., Lin, L.-C. & Poloni, R. "Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metal–Organic Frameworks". *Chemistry – A European Journal* **24,** 15167–15172 (2018).
- **Kshirsagar**, A. R. "First-Principles Investigation of MoS2-MXene Heterostructures as Cathodes in Magnesium Ion Batteries. M.S. Thesis". *Indian Institute of Science Education and Research, Pune* (2017).

## TEACHING EXPERIENCE

**Initiation to Research, Energy in Chemistry : 27 hours**
*The undergraduate course comprised of 3h ($\times 2$ batches) lectures on Quantum Chemistry and hands-on training of calculations of formation energies of molecules and analysis of chemical bonding in terms of quantum interference of atomic orbitals.*

**Cycle pluridisciplinaire d'etudes supérieures (CPES), University of Rennes**

2025-26 Rennes, France

**In-charge**: Xavier Rocquefelte

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**Tutoring in VASP workshop : 15.5 hours**
*The workshop comprised of theoretical and hands-on training on density-functional-theory (DFT) calculations using the Vienna Ab-initio Simulation Package (VASP)*

**University of Rennes and VASP Software GmbH**

2025 Rennes, France

**In-charge**: Xavier Rocquefelte

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**Mentorship of Masters students: 12 hours**
*A short research project on determination of molecular structures using density functional theory*

**Functionalized Advanced Materials Engineering (FAME+) European Masters program, Grenoble-INP, University of Grenoble-Alps**

2020-2021 Grenoble, France

**In-charge**: Roberta Poloni

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**Mentorship of Masters students: 6 hours**
*A short research project on optimisation of structure of porous materials using density functional theory*

**Phelma engineering school, Grenoble-INP, University of Grenoble-Alps**

2019-2020 Grenoble, France

**In-charge**: Roberta Poloni **Co-supervisor**: Lorenzo A. Mariano

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**Mentorship of school science club**
*Conducting science workshops for school students*

**Dr. Vasantdada Patil Municipal School, K. C. Thackeray Municipal School**

2014-2016 Pune, India

**In-charge**: Shraddha Gargatti, Exciting Science Group

## ORGANISATIONAL EXPERIENCE

- Organisation of weekly seminars in Theoretical Inorganic Chemistry Unit at ISCR
  2025 — Rennes, France
- Assistant for symposium *Halide perovskites for quantum technologies* at MATSUS Spring
  April 2025 — Sevilla, Spain
- Committee member of LuxDoc, an association of nonpermanent researchers
  2022-2023 — Luxembourg
- Co-organizer of the annual workshop of department of physics and materials science (DPhyMS)
  2022 — Luxembourg
- Co-organizer of 'Rencontres des Jeunes Physicien(ne)s' (Young Physicists' Meet)
  2017 — Grenoble, France
- Part of organizing team of March for Science
  2017 — Pune, India
- General coordinator of 'Mimamsa', pan-India undergraduate science quiz
  2015 — Pune, India

## SKILLS

### Computer skills

Python | Matplotlib | Numpy | Fortran (basics) | Linux | High performance computing | Bash | Numerical methods | QuantumEspresso | Abinit | SIESTA | Yambo | Wannier90 | NWChem | Orca | Office | LaTeX | Inkscape

### Scientific skills

Quantum mechanics | Quantum chemistry | Solid state physics | Atomistic modeling | Computational material science | Material characterisation | Density functional theory | Molecular dynamics | Structure optimisation | Perturbation Theory | Bethe-Salpeter Equation | Density functional perturbation Theory | Optical spectroscopy | Vibrational spectroscopy | Electronic excitations | Group theory | Chemical bonding | Data analysis | Connecting experiments to theory

### Communication skills

Science communication | Article and report writing | Data visualization | Presentation skills | English: C1 | French: B1 | Hindi: C1 | Marathi: Native

## ACHIEVEMENTS

Selected for 'Make Our Planet Great Again' (MOPGA) one-year visiting fellowship program
2025 — Campus France, French Government

Research fellowship by qualifying National Eligibility Test in Physics with all India rank 78
2016 — Council of Scientific and Industrial Research (India)

INSPIRE undergraduate scholarship
2012-17 — Department of Science and Technology, India

## CONFERENCES

ThéMoSiA: West Pole meeting

***Talk: Theoretical description of circular dichroism in solids: new directions***

Dec 2025 — Nantes, France

Psi-K 2025

***Poster: Interplay of charge, spin, and lattice via on-site excitons in multiferroic perovskite***

Aug 2025 — Lausanne, Switzerland

Chiral Phonons workshop, Johannes Gutenberg University Mainz

***Poster: Chirality transfer in hybrid organic-inorganic materials : role of chiral vibrational modes***

Jul 2025 — Ingelheim, Germany

Journées Pérovskites Halogénées, CNRS GDR

***Poster: Modulation of magnetization in BiFeO3 using circularly polarized light***

Mar 2025 — Erquy, France

Young Investigator's Meet on Quantum Condensed Matter Theory, IISER Pune

***Invited talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

Dec 2024 — Pune, India

International Workshop on 2D Heterostructures (HOWDI)

***Poster: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

Oct 2024 — Lipperscheid, Luxembourg

March Meeting of American Physical Society (APS)

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

March 2024 — Minneapolis, United States of America

International Winter School 2023, Jawaharlal Nehru Centre for Advance Scientific Research

***Poster: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

December 2023 — Bengaluru, India

GDR-REST: Rencontres de Spectroscopie Théorique (Theoretical Spectroscopy Meeting)

***Talk: Resonant coupling of spin-flip excitations with phonons in $BiFeO_3$***

June 2023 — Île d'Oléron, France

German Physical Society (DPG) spring meeting

***Talk: Resonant coupling of spin-flip excitations with phonons in $BiFeO_3$***

March 2023 — Dresden, Germany

EPW 2022: Summer School on Electron-Phonon Physics from First Principles

***Poster: First-principles study of resonant Raman scattering in $BiFeO_3$***

June 2022 — Austin, United States of America

JTMS 2020: Journées Théorie, Modélisation et Simulations (organized by French Phys. Soc. and French Chem. Soc.)

***Talk: Optical properties of photoresponsive MOFs: assessing fragment models using the BSE/GW formalism***

Nov 2020 — Online, France

MOFSIM 2019

***Poster: First-principles investigation of photo-responsive metal-organic-frameworks for efficient CO2 capture***

Apr 2019 — Ghent, Belgium

Theoretical Spectroscopy Lectures

***Poster: First-principles investigation of photo-responsive metal-organic-frameworks for efficient CO2 capture***

Oct 2018 — Lausanne, Switzerland

Journée de la Matière Condensée (organized by French Physical Society)

***Poster: First-principles investigation of photo-responsive metal-organic-frameworks for efficient CO2 capture***

Aug 2018 — Grenoble, France

GDR-REST: Rencontres de Spectroscopie Théorique

***Talk: First-principles investigation of photo-responsive metal-organic-frameworks for efficient CO2 capture***

May 2018 — Porquerolles, France

## INVITED TALKS

Tata Institute of Fundamental Research — Host: Dr. Darshan Joshi

***Talk: Chiral Quantum States: Interplay of Spin, Charge and Lattice***

Nov 2025 — Hyderabad, India

Institute of Chemical Technology, Mumbai — Host: Dr. Ashwin Mohan

***Talk: Light-induced processes in materials : insights from ab initio methods***

Jan 2025 — Mumbai, India

Institute of Physics and Chemistry of Materials of Strasbourg (IPCMS) — Host: Prof. Mébarek Alouani

***Talk: Light-induced processes in materials : insights from ab initio methods***

March 2024 — Strasbourg, France

Institute Charles Gerhardt Montpellier (ICGM) — Host: Dr. Guillaume Maurin

***Talk: Light tunable gas adsorption in functionalised metal-organic frameworks: insights from ab initio methods***

February 2024 — Montpellier, France

Laboratory Charles Coulomb — Host: Dr. Thibault Sohier

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

February 2024 — Montpellier, France

Institute of Chemical Sciences of Rennes (ISCR), University of Rennes — Host: Dr. Claudine Katan

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

February 2023 — Rennes, France

Institute of Electronics, Microelectronics and Nanotechnology (IEMN) — Host: Dr. Christophe Delerue

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

January 2023 — Lille, France

Indian Institute of Science Education and Research (IISER), Pune — Host: Dr. Prasenjit Ghosh

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

December 2023 — Pune, India

Institute of Molecules and Materiels of Le Mans — Host: Dr. Mads Weber

***Talk: Modulation of magnetization in $BiFeO_3$ using circularly polarized light***

November 2023 — Le Mans, France

University of Liège — Host: Prof. Matthieu Verstraete

***Talk: Understanding excitons in $BiFeO_3$***

April 2023 — Liège, Belgium

Interdisciplinary Center of Nanoscience of Marseille — Host: Dr. Claudio Attaccalite

***Talk: Ab initio study of photo-responsive metal-organic frameworks for an efficient carbon capture***

January 2020 — Marseille, France

## PEER-REVIEW ACTIVITY

Physical Review Letters, Physical Review B, Physical Review Materials (American Physical Society)

2024-present

## OTHER AFFILIATIONS

- Member of American Physical Society, APS (2023-2024)
- Member of German Physical Society, DPG (2022-2024)
- Member of European Theoretical Spectroscopy Facility, ETSF (2022-present)