Dr. Aleena Alex
MSCA-COFUND post-doctoral fellow (ADAGIO fellowship)
University of Basque Country (UPV/EHU), Spain
Visiting Researcher, Newcastle University, United Kingdom
aleena.alex@ehu.eus, aleena.alex@newcastle.ac.uk
https://www.researchgate.net/profile/Aleena_Alex2

Academic Education and Qualifications

Degree	Institute/Organization	Thesis or Dissertation Topic	Year and Score
PhD (Applied Mechanics)	Indian Institute of Technology Madras, Chennai, India.	An interface based multi-scale mechanical model for cementitious materials	2014-2020 **CGPA: 9.23/10**
Master of Technology **(MTech) in Engineering of Structures**	Academy of Scientific and Innovative Research (AcSIR), Council of Scientific and Industrial Research (CSIR), Chennai, India.	Evaluation of Engineering Properties of Cement Clinkers using Molecular Dynamics	2012-2014 **CGPA: 9.22/10**
Bachelor of Technology **(BTech) in Civil Engineering**	National Institute of Technology Calicut, Kerala, India.		2008-2012 **CGPA: 9.04/10**

Research Interests

Carbonation/mineralization, Biomineralization, Self-healing concrete, Cement Chemistry, Multiscale modelling, Molecular Dynamics, kinetic Monte Carlo, Finite Element Analysis, Nanomechanical characterization of materials, Spectroscopy, Computational materials modelling.

Research Experience

Jan 2023-	**Marie Sklodowska Curie Actions (MSCA) fellow,** University of Basque Country (UPV/EHU), Spain **Host**: Prof. Hegoi Manzano • Modelling molecular dissolution and precipitation of C-S-H, M-S-H and $CaCO_3$ using Kinetic Monte Carlo (KMC)
Sep 2023-Apr 2024	**Visiting Researcher,** Newcastle University, UK • C-DICE proof of concept grant TASTES-Techno-economic Assessment of dispersed sites with Thermal Energy Storage in the UK
March 2021-Aug 2023	**Research Associate,** Newcastle University, UK **Supervisors:** Dr. Dana Ofiteru • Impact Acceleration project: Bacteria based self-healing of concrete in wastewater
May 2021-Feb 2023	**Research Associate,** Newcastle University, UK **Supervisors:** Dr. Dana Ofiteru, Dr. Enrico Masoero • A Kinetic Monte Carlo framework was used to model autogenous healing in mineral systems by simulating calcium carbonate precipitation. • The nano-scale mineral system is coarse-grained to micro-scale.

	• The 2 C++ code bases, both working on LAMMPS platform, MASKE handling dissolution and precipitation of mineral and NUFEB handling growth and division of bacteria are combined. • Mineral dissolution-precipitation individual based model (IBM) combined with bacterial growth-metabolism IBM.
July 2014-July 2020	**Research Scholar,** Indian Institute of Technology, Madras **Advisor:** Dr. Pijush Ghosh, Professor • Developed a multiscale mechanical model for cement, based on discrete lattice spring mechanics to evaluate the mechanical properties of hydrating cementitious materials such as C_3S and C_2S. • A combination of nanomechanical characterisation techniques (nanoindentation and SEM imaging) and both discrete and continuum scale simulations were employed for the development of the model. • Chemical analysis of cementitious materials using Raman spectroscopy, FTIR, SEM/EDAX etc. • Applied and validated the multiscale model developed for different systems such as varying percentage combinations of C_3S and C_2S and C_3S combined with silica nanoparticles. • Explored biodegradation behaviour of Polylactic acid (PLA) decoupling the effect of solvation and hydrolysis using a combination of experimental analysis (nanoDMA) and MD simulations. • Studied the effect of mineral surfaces (C_3S/C_2S) on confined water using molecular dynamic simulations.
Sep 2012 – July 2014	**Trainee Scientist**, CSIR Structural Engineering Research Centre **Advisor**: Dr. Saptarshi Sasmal, Senior Principal Scientist and Head, CSIR-SERC • Evaluated the mechanical properties of cement clinkers (C_3S, C_2S, C_3A) using molecular dynamic simulations. • Compared the effect of different forcefields and interaction potentials on the mechanical property estimation and load displacement characteristics. • Developed finite element codes for solving complex static and dynamic problems such as uni-axial deformation in truss, beam bending (plane stress, plane strain), deformation of plates (Kirchoff and Mindlin), meshfree techniques etc.

Teaching Experience

Lecturer for a module in the post graduate course, Water Supply and Treatment - CEG8103 (Module leader: Dr. Russell Davenport) at Newcastle University.

Lecturer for the viscoelastic models and nanoDMA module for the class of postgraduate students as part of the course Nanomechanics and Nanomaterials at IIT Madras.

Teaching Assistant undergraduate (Engineering Mechanics, Strength of Materials), postgraduate (Applications of Molecular Dynamics, Nanomechanics and Nanomaterials) and laboratory courses (Contact angle and surface energy).

Conducted tutorial/practice session on Engineering Mechanics and Strength of Materials for a group of 120 undergraduate students.

Conducted tutorial/practice session on MD simulator (LAMMPS/VMD/Packmol) for a group of 30 postgraduate students.

Awards & Grants

Awarded **Marie Sklodowska Curie Actions (MSCA)-COFUND fellowship** as part of the ADAGIO programme at University of Basque country (UPV/EHU), Spain with secondment at Politecnico di Milano, Italy. The fellowship is hosted by Prof. Hegoi Manzano.

Won **28000 GBP proof of concept grant** with Dr. Xin Liu, University of Nottingham, at the Dispersed Industrial Decarbonisation sandpit conducted by Centre for Post-doctoral development in infrastructure cities and energy (**C-DICE**).

Secured **AWSAR Award** for best popular science story conducted by Department of Science and Technology for the year 2019-2020.

Secured full fee waiver and travel grant (1200 EUR) from Heidelberg University, Germany to attend and deliver contributed talk at the Summer School *"Mathematical Modeling in Quantum Chemistry"* organized by Interdisciplinary Centre for Computational Sciences (IWR), on 2-6th October 2017.

Awarded **Best Poster Award** for the work entitled *"Application of Nanomechanical Properties in Developing the Multiscale Model of Hydrating Cement Interfaces"* at the conference, Nanoyantrika-2017 held at Trivandrum-India on 17th-19th September 2017.

Secured Indian Institute of Technology Madras (IITM) Institute travel grant (1,50,000 INR) to attend and deliver contributed talk at RILEM SMSS 2019, 18th -22nd March 2019, Rovinj, Croatia.

Secured Indian Institute of Technology Madras (IITM) Alumni travel grant (50,000 INR) to attend and deliver contributed talk at Computational Modelling of Concrete Structures (EURO-C 2018), 26th February-1st March 2018, Bad Hofgastein, Austria.

Secured Half-time Teaching Research Assistantship (HTRA) funded by MHRD, India while pursuing PhD at IIT Madras. The award provided a monthly stipend (28,000 INR/mo) during 5 years of PhD.

Secured fully funded Trainee Scientist position at CSIR-SERC to pursue master's degree. The award provided a monthly stipend (35,000 INR/mo) during 2 years of MTech.

Skills & Activities

Computational Skills	Molecular Dynamics Simulation, Finite Element Analysis, Discrete Element Modelling, Kinetic Monte Carlo simulations
Software Skills	LAMMPS, VMD, Packmol, Material Studio, Matlab, C++
Experimental Skills	Nanoindentation, NanoDMA, Nanoscratch, FTIR, Contact angle and Surface Tension Analysis, Micro indentation, Raman spectroscopy

Memberships

RILEM Technical committee member: Data driven Concrete Science (DCS), Accelerated Mineral Carbonation for the production of construction materials (MCP)

Publication Highlights

Journal Publications

1) Aleena Alex, Brubeck Freeman, Anthony Jefferson, Enrico Masoero, "Carbonation and self-healing in concrete: Kinetic Monte Carlo simulations of mineralization" **Cement and Concrete Composites** (2023): 105281

2) Bagga, Manpreet, Charlotte Hamley-Bennett, Aleena Alex, Brubeck L. Freeman, Ismael Justo-Reinoso, Iulia C. Mihai, Susanne Gebhard et al. "Advancements in bacteria based self-healing concrete and the promise of modelling." **Construction and Building Materials** 358 (2022): 129412.
3) Aleena Alex, Nirrupama Kamala Ilango, and Pijush Ghosh. Interface microstructure based mechanical property evaluation of C-S-H. **Journal of Materials in Civil Engineering** 35.2 (2023): 04022431
4) Nirrupama Kamala Ilango, Pratik Gujar, Ashwin Konanur Nagesh, Aleena Alex, and Pijush Ghosh. Interfacial adhesion mechanism between organic polymer coating and hydrating cement paste. **Cement and Concrete Composites** 115 (2021): 103856.
5) Pratik Gujar, Aleena Alex, Manu Santhanam, and Pijush Ghosh. Evaluation of interfacial strength between hydrating cement paste and epoxy coating. **Construction and Building Materials** 279 (2021): 122511.
6) Ashwin Konanur Nagesh, Nirrupama Kamala Ilango, Aleena Alex and Pijush Ghosh. Effect of pore solution calcium and substrate calcium on PMMA/cement paste interface during early stages of hydration. **Journal of the American Ceramic Society** 103.8 (2020): 4664-4677.
7) Aleena Alex, Nirrupama Kamala Ilango, and Pijush Ghosh. Comparative Role of Chain Scission and Solvation in the Biodegradation of Polylactic Acid (PLA). **The Journal of Physical Chemistry B** 122.41 (2018): 9516-9526.
8) Aleena Alex, Ashwin Konanur Nagesh, Pijush Ghosh: *Surface dissimilarity affects critical distance of influence for confined water*. **RSC Advances** 01/2017; 2017(7)., DOI:10.1039/c6ra25758e
9) Aleena Alex, B S Sindu, Saptarshi Sasmal: *Uniaxial Tension and Compression Studies on Cement Clinkers Using Molecular Dynamic Simulations.* **Journal of Structural Engineering**; Vol. 42, No. 1, Apr - May 2015 pp. 22-27
10) B S Sindu, Aleena Alex, Saptarshi Sasmal: *Studies on structural interaction and performance of cement composite using Molecular Dynamics.* **Advances in Computational Design (Techno Press);** Vol. 3, No. 2, 2018, pp 147-163, DOI: 10.12989/acd.2018.3.2.147

International Conferences

1) Aleena Alex, Enrico Masoero and Dana Ofiteru, *Carbonation in bacteria based self-healing cement: A new modelling approach*, **Keynote Lecture** at Discrete Models for Material Failure mini-symposium, part of **CFRAC-2023**, Prague.
2) Enrico Masoero, Aleena Alex and Dana Ofiteru, *Kinetic Monte Carlo simulations of carbonation and self-healing in concrete*, **ECCOMAS Congress 2022**, 5th to 9th June 2022, Oslo, Norway.
3) Aleena Alex, and Enrico Masoero, *Autogenous healing in cement: a kinetic Monte carlo simulation of $CaCO_3$ precipitation,* Computational Modelling of Concrete Structures (**EURO-C 2022**), 22nd-26th May 2022, Vienna, Austria.
4) Aleena Alex and Pijush Ghosh, *An approach towards the multiscale modelling of hydrating cement matrix,* **RILEM SMSS 2019**, 18th -22nd March 2019, Rovinj, Croatia.
5) Aleena Alex and Pijush Ghosh, *Multiscale mechanical model of hydrating C_3S*, 3rd R.N. Raikar Memorial International Conference and Gettu-Kodur International Symposium on **Advances in Science and Technology of Concrete**, 14th - 15th December 2018, Mumbai, India.
6) Aleena Alex, and Pijush Ghosh, *Modeling the evolution of C_3S-C_3S grain interface over hydration time,* Computational Modelling of Concrete Structures (**EURO-C 2018**), 26th February-1st March 2018, Bad Hofgastein, Austria.
7) Aleena Alex and Pijush Ghosh, *Temporal Evolution of Microstructure, Chemical and Mechanical Properties of Tricalcium Silicate*. International Conference on Advances in Construction Materials and Systems (**ICACMS-2017**), 3rd -8th September 2017, Chennai, India.
8) Aleena Alex and Pijush Ghosh: *A Molecular Dynamics study on the effect of Dicalcium and Tricalcium Silicate surfaces on the structure of water*. **UKIERI Concrete Congress**, 2nd-5th November 2015, NIT Jalandhar, India.
9) Aleena Alex, Sindu B. S and Saptarshi Sasmal: *Uniaxial Tension and Compression Studies on Cement Clinkers Using Molecular Dynamic Simulations*. International Conference on Computational Mechanics and Simulation (**ICCMS-2014**)-10th -13th December 2014, CSIR-SERC Chennai, India.