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IGSTC PhD Industrial Exposure Fellowship: Project I

Title: Modeling the Impact of Chemical Admixtures on the Hydration of Environmentally Friendly Low-Clinker Cement

Description: We are looking for a highly motivated candidate to join our Group "Quantum Chemistry & Molecular Modeling" within the Group Research division. In this role, you will play a crucial part in the development of sustainable construction technology for low-clinker cement in the construction industry among others. Using advanced molecular modeling techniques, you will work on predicting the interactions of cement surfaces with different chemical additives to understand their performance based on rheological and thermodynamic properties. You will also gain experience in designing effective chemical additives for low-CO_2 cement-based materials.

Your responsibilities will include optimizing all-atom models of hydrated cement surfaces to perform accurate MD simulations of cement surface interactions with chemical admixture in the pore solution. The models should be able to predict the adsorption behavior of different polymers on various hydrated cement surfaces, which is crucial in designing effective chemical admixtures. Additionally, you will learn how to use the LAMMPS, Gromacs, Interface field model validation workflows in combination with the EMC (Enhanced Monte Carlo Structure Generator) software (https://montecarlo.sourceforge.net/emc/Welcome.html), umbrella sampling using SSAGES and GROMACS and create the coarse-grain parameterizations for mineral-organic interfaces.

Minimum education and skillsets:

- Currently enrolled in a PhD program that includes materials molecular modeling, preferentially with focus on all-atom force field development, computation of adsorption free energy and exposed to coarse-grained MD simulations.
- Familiar with Linux OS, MD simulations using LAMMPS, visualization using VMD, Data analysis, Python programming.
- Intrinsic self-motivation and ability to work independently.
- Passionate about interfacial chemistry and proactive in implementing creative ideas.
- Excellent organizational skills and ability to thrive in an international environment.

*Kindly note that the skillsets required by BASF are over and above the eligibility criteria of IGSTC PhD Industrial Exposure Fellowships. PhD students who wish to get a Letter of Consent while applying to IGSTC Industrial fellowships are advised to contact BASF personnel if and only if they satisfy the above conditions.

Please send your resume and cover letter for this position to igstc.application@basf.com with "IGSTC Industrial Fellowships 2025" in the subject of the email. Kindly note that an application without cover letter addressing skillset and motivation to join this project may be rejected without any notification.

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IGSTC Post-Doctoral Industrial Fellowship: Project I

Title: Enabling Modeling Methods for Adhesion between Inorganic-Organic Interfaces

Description: We are looking for a highly motivated candidate to join our Group "Quantum Chemistry & Molecular Modeling" within the Group Research division. In this role, you will play a crucial part in the development of sustainable surface pretreatment technology for metal oxide and recycled alloy surfaces in industries such as automotive, aerospace, and construction. Additionally, you will work on a project involving chemical admixtures for low-clinker cement in the construction industry. This role offers the opportunity to collaborate with a diverse team of scientific experts to drive innovative solutions.

Your responsibilities will include optimizing all-atom models of inorganic mineral surfaces to perform accurate MD simulations of surface interactions with polymeric additives in the solution. Your research focus will be on predicting polymer adsorption on various mineral surfaces at different pH levels, essential for creating effective coatings, nanocomposites, and chemical admixtures. Additionally, you will use the LAMMPS, Gromacs, Interface field model validation workflows in combination with the EMC (Enhanced Monte Carlo Structure Generator) software (https://montecarlo.sourceforge.net/emc/Welcome.html), umbrella sampling using SSAGES and GROMACS and create the coarse-grain parameterizations for inorganic-organic interfaces.

Minimum education and skillsets:

- A recent PhD in atomic-scale simulations for inorganic-organic interfaces that includes materials molecular modeling, preferentially with focus on machine learning techniques, all-atom force field development, and exposed to multiscale modelling approaches.
- Familiar with Linux OS, MD simulations using LAMMPS, visualization using VMD, Data analysis, Python programming.
- Intrinsic self-motivation and ability to work independently.
- Passionate about interfacial chemistry and proactive in implementing creative ideas.
- Excellent organizational skills and ability to thrive in an international environment.

*Kindly note that the skillsets required by BASF are over and above the eligibility criteria of IGSTC Post-Doctoral Industrial Fellowship. Candidates who wish to get a Letter of Consent while applying to IGSTC Industrial fellowships are advised to contact BASF personnel if and only if they satisfy the above conditions.

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