

Understanding Cold-Water Coral Strength: Molecular Interactions and Scaling Simulations



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Abstract: Understanding cold-water coral strength: Molecular interactions and scaling simulations", and the abstract: "Cold-water corals exhibit complex hierarchical structures composed of aragonite crystals and organic interfaces. Understanding their mechanical behaviour requires modelling at different length scales. In this talk, we use Molecular Dynamics (MD) simulations to characterize aragonite crystal behaviour, twin boundaries, and interactions with proteins. Coarse-Grained (CG) models are then developed to capture larger-scale behaviours while preserving key mechanical properties. Our approach refines the interatomic potentials for aragonite-protein interactions, ensuring an accurate representation of the tensile and shear properties. The transition from MD to CG modelling is achieved through parameter fitting, allowing an efficient yet accurate description of mesoscale mechanical responses. We further explore the role of water-mediated interactions, nanoporosity, and structural anisotropy in influencing the mechanical response of corals.

Biography: Nikolai is a postdoctoral researcher at TU Clausthal, working on multiscale modelling of biomineral materials. He completed his Master's degree at the St. Petersburg Polytechnic University and obtained his PhD at the Polytechnic University of Catalonia. His PhD research focused on slip transfer mechanisms in bcc metals, particularly the interaction of lattice defects in iron. Currently, he is extending these concepts to biomineralized tissues, exploring the mechanics of aragonite-organic materials systems through molecular dynamics, coarse-grained simulations, and finite element approaches

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