CHYN MEETS HARBOR

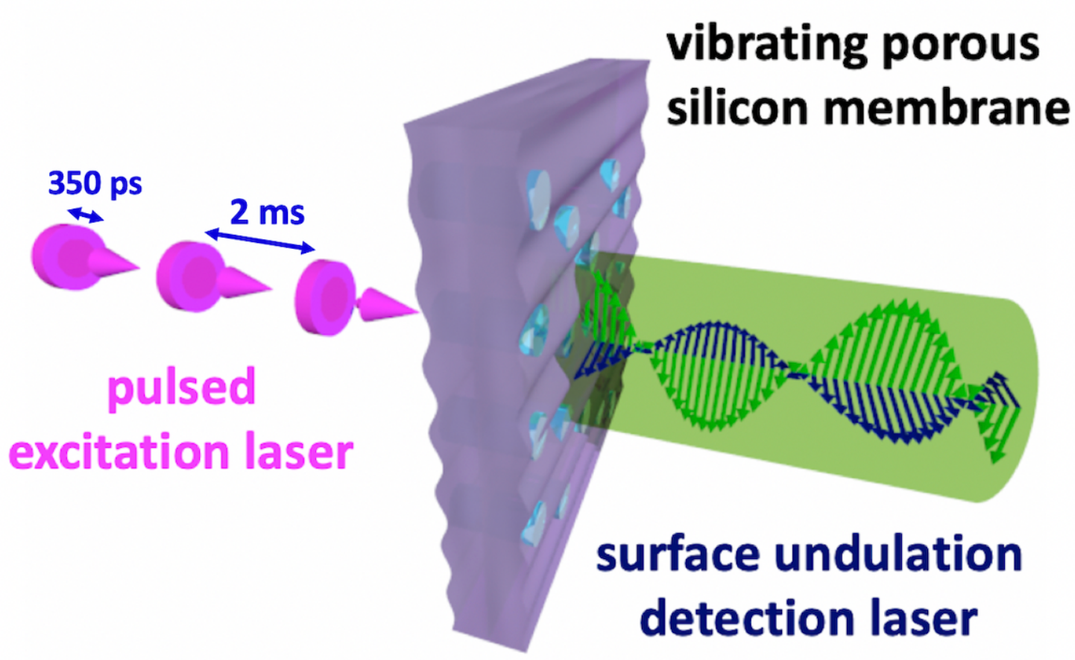
Laser-excited elastic guided waves reveal the complex mechanics of nanoporous silicon

Marc THELEN

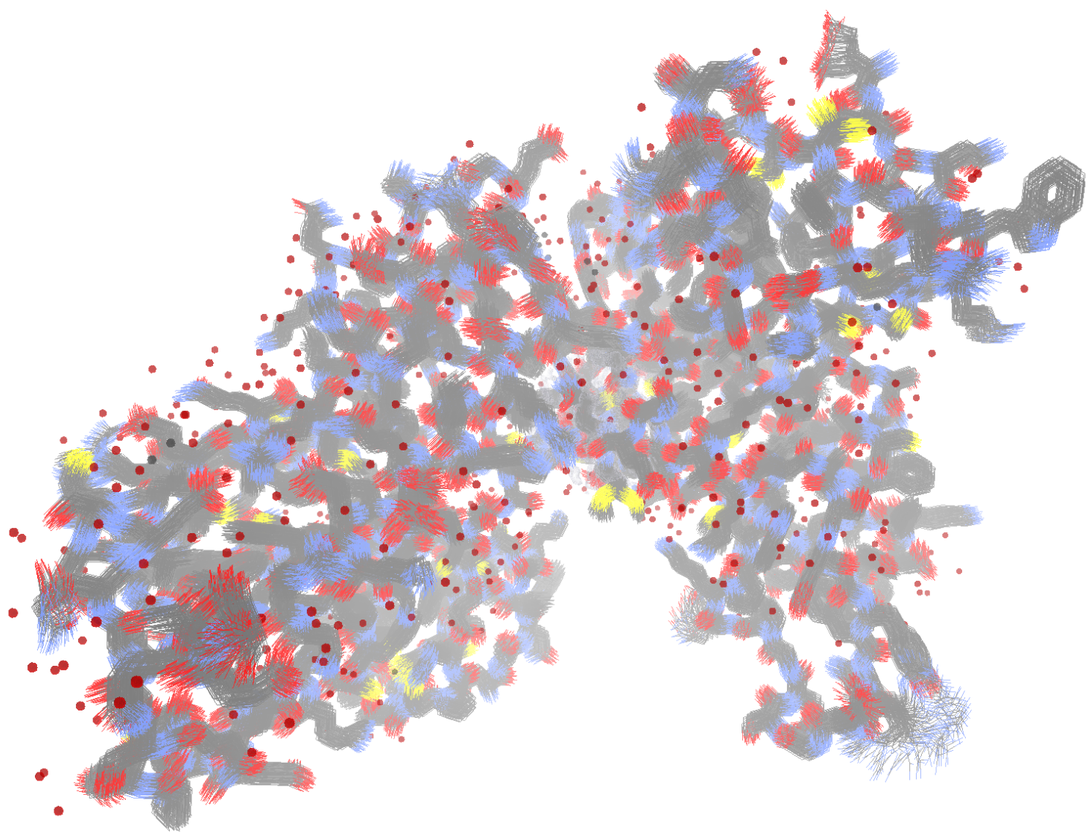
Vagabond: A software package for protein model refinement

Dr. Helen GINN

Abstract Talk 1: Nanoporosity in silicon leads to completely new functionalities of this mainstream semiconductor. A difficult to assess mechanics has however significantly limited its application in fields ranging from nanofluidics and biosensorics to drug delivery and energy storage. Here, we present a study on laser-excited elastic guided waves detected contactless and non-destructively in dry and liquid-infused single-crystalline porous silicon. These experiments reveal that the self-organized formation of 100 billions of parallel nanopores per square centimeter cross section results in an isotropic elasticity perpendicular to the pore axes and an 80% stiffness reduction in the material, despite a bulk-like and anisotropic pore-wall elasticity. Our complete assessment of the wafer-scale mechanics of nanoporous silicon provides the base for predictive applications in robust on-chip devices and evidences that recent breakthroughs in laser ultrasonics open up entirely new frontiers for in-situ, non-destructive mechanical characterisation of dry and liquid-functionalised porous materials.



Abstract Talk 2: Model refinement for biomolecular crystallography relies on a model defined in atomic x, y, z parameters and associated B factors. The talk will summarise the state-of-the-art methodology in model refinement and its historical basis. I shall go on to introduceVagabond, a new refinement project which revisits the concept of refining in torsion space, defining the model in terms of bond lengths, angles and torsion angles. This significantly reduces the number of parameters required to describe most of the structure. However, it also incorporates a novel model for expressing flexibility in a chemically sensible manner, and is capable of describing weird and wonderful atomic distributions which are not accessible from isotropic or anisotropic B factor models. The combination of these features leads to a reduction in overfitting and increased clarity of maps.



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