

# **Accurate Retrieval of Three-Dimensional Atomic Dynamics of Moiré Materials**

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Determination of the three-dimensional (3D) atomic positions of materials is the key factor to understand the physical properties. Visualization of 3D atomic structure of nano-scale crystalline objects has been demonstrated from in-line holography by low dose rate electron microscopy. However, this method needs to resolve individual atom column along projection of electron beam. Here, an analytic method based on simulated annealing and energy minimization algorithms is proposed to retrieve the 3D atomic dynamics of moiré materials, such as single-walled carbon nanotube and twisted bilayer graphene, in which atomic column is not well-resolved and moiré fringe exists. The accurate determination of atomic positions can reveal the detailed structural properties, such as deformation field and surface roughness. This ability to probe structural change in time series is pivotal to understand the structure-function relationship of nanomaterials.