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Probing Chemical and Geometrical Properties of Crystal Surfaces with First Passage Times

The statistics of first passage times (FPT) is used widely in the field of statistical physics. In this work, we study the FPT distributions of water near three different crystal surfaces of the amino acid glutamine. We show that each surface leaves a unique fingerprint of the structural and geometrical properties of crystal in the FPT distributions. We also establish a theoretical model for the FPT in bulk water using a simple Langevin dynamics, hence providing a framework to understand water fluctuations near proteins.

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