Temple University Mathematics Colloquium

Pak-Wing Fok

University of Delaware

will speak on

Reconstruction of bond potentials from multiple rupturing time data

ABSTRACT: We explore the reconstruction of the functional form of the potential energy surface of a molecular bond from distributions of its rupture times. For a single measured first passage time (FPT) distribution the inverse problem is ill-posed and only a few attributes (such as the height and width of an energy barrier) can be reconstructed.

However, reconstruction of finer details of the bond potential can be achieved by simultaneously using two or more measured FPT distributions, obtained under different physical conditions. For example, by changing the potential energy surface by known amounts, the additional FPT distributions render the inverse problem less ill-posed. We demonstrate the feasibility of reconstructing potential with multiple minima, motivate general rules for optimizing the reconstruction, and discuss further applications and extensions.

Monday, 9 November 2009
Lecture at 4:00 pm
Coffee, tea, and refreshments from 3-5 pm
Room 617, Wachman Building
Department of Mathematics