



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
COLLOQUIUM

Non-equilibrium Exciton Dynamics in Solids: A First-Principles Perspective

by



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Time: 3:00 - 4:00 p.m.

Place: L2, Science Centre, CUHK

(Light refreshments will be served at [SCNB 1/F lobby](#) from 2:30 to 2:50 p.m.)

ALL INTERESTED ARE WELCOME

Abstract

Understanding nonequilibrium quasiparticle dynamics in materials requires going beyond static electronic structure. Here, we present an ab initio framework that combines GW/BSE with real-time quantum dynamics to simulate exciton dynamics in different materials. It is shown that exciton dynamics is fundamentally driven by different many-body interactions. In transition metal dichalcogenides, exchange interaction enables ultrafast valley depolarization by opening intervalley channels forbidden in a single-particle picture. Furthermore, phonons act as a dynamical switch that activates long-range Coulomb coupling, leading to rapid bright-to-dark exciton relaxation. When electron-phonon coupling are strong enough, it can also dress the exciton and form polaron-exciton in polar materials. We reveal the formation of dynamically fluctuating polaron-exciton states in TiO_2 , where electron-phonon coupling and Coulomb interaction cooperatively determine the quasiparticle properties and lifetimes.

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