

Joint CQSE and CASTS Seminar

Weekly Seminar
Jun. 8, 2012 (Friday)

TIME Jun. 8, 14:30 ~ 15:30
TITLE Probing Many-Body Effects in Low-Dimensional
Nanomaterials: Ab-initio Study
SPEAKER Prof. Hung-Chung Hsueh
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Abstract

Many-body interactions are known to be the essential issue of a wide variety of material systems, especially in low-dimensional nanomaterials due to their structural dimensionality effects. Other than recent tremendous advances in modern experimental techniques, quasiparticle many-body perturbation theory within a GW approximation plus solving Bethe-Salpeter equation (GW+BSE) and time-dependent density functional theory (TDDFT) with specially tuned approximation are two main first-principles methods beyond mean-field approximation to probe the many-body effects in materials. Providing an intuitive physical picture and deeper understanding of the many-body problem, GW+BSE method has been therefore performed in the present work to explore the unique electronic and optical properties of semiconducting mono/few-layer nanosheets and single-walled nanotubes. Comparing with conventional bulk systems, our results showed that huge excitonic effects in nanosystems are attributed to the significant reduced charge screening and enhanced electron-electron correlation. Meanwhile, effective cancellation of electron-hole/ electron-electron interaction in these low-dimensional materials was also discussed.

