

MANY-BODY QUANTUM CHEMISTRY FOR CON-DENSED PHASE SPECTRA

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California Institute of Technology, Pasadena, CA, U.S.A. The first principles computation of the single-particle and optical spectra of solids provides one of the most direct ways to link theory and experiment. However, quantitatively accurate spectra have been hard to obtain in more correlated materials, due to the difficulties in treating interactions. I will describe how modern methods of quantum chemistry are now poised to provide a systematically improvable and high-accuracy framework to compute electronic spectra in correlated materials.

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CFEL SEMINAR ROOMS I-III

















