

# Optical excitations and spectroscopic properties of nanostructures and organic molecules from first-principles Green's function methods

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Since the last twenty years, Green's function techniques have been successfully used to predict various spectroscopic and optical properties of real materials. The core of these techniques resides in two ingredients: evaluating the electron self-energy within the so-called GW approximation; and solving the Bethe-Salpeter equation for charge-neutral (optical) excitations. Despite the success of these techniques in periodic systems, there has been little work in non-periodic systems such as nanocrystals and organic molecules. In order to fill out this gap, we have developed a numerical implementation of Green's function methods in the space of electron-hole pair transitions. This is particularly useful and surprisingly efficient in non-periodic or partially periodic systems. With this implementation, we could study the optical properties of silicon nanocrystals containing more than one hundred atoms. We have also applied it to cadmium selenide and gallium arsenide nanocrystals, organic and inorganic molecules. Predictions of Green's function methods are compared to other theoretical approaches and with available experimental data.