Excited calculations of large scale multiwalled nanotubes using real-space pseudopotential methods

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One method for calculating excited states is the GW method. The GW method has many computational requirements. One of the bottlenecks is the calculation of numerous empty states. Within density functional theory, we use a real-space pseudopotential method (PARSEC) to calculate these empty states for multiwalled nanotubes. We illustrate the use of these empty states for calculating excited states using the GW method (BerkeleyGW). We demonstrate why using real-space density functional theory is advantageous for calculating empty states.

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