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Excited calculations of large scale multiwalled nanotubes using real-space pseudopotential methods[1] CHARLES LENA, JAMES CHELIKOWSKY, University of Texas at Austin, JACK DESLIPPE, National Energy Research Scientific Computing Center, YOUSEF SAAD, University of Minnesota, CHAO YANG, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — 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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