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On the accuracy of the G^0W^0 method: From Si to ZnO[1] PEIHONG ZHANG, ZHIJUN YI, BI-CHING SHIH, Department of Physics, University at Buffalo, State University of New York, Buffalo, New York 14260, JACK DESLIPPE, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — The *ab initio* GW method has been recognized as one of the most powerful theories in predicting quasiparticle excitations in solids. Due to computational limitations, earlier GW calculations usually made use of certain generalized plasmon-pole approximations to carry out frequency integration of the electron self-energy. In addition, often the convergence of the calculated results with respect to various cutoff parameters (such as the number of conduction bands and the size of the dielectric matrix) was not investigated in details. With advances in computational methodology and technology, fully converged GW calculations with explicit frequency integration become possible. In this talk, we will discuss fully converged G^0W^0 results for a range of materials, ranging from the most "theory friendly" system Si to the widely discussed and controversial system ZnO. We will compare explicit frequency integration vs various generalized plasmon-pole models. We will also discuss effects of various cutoff parameters used in GW calculations.

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Bi-Ching Shih
Dept of Physics, University at Buffalo, State University of New York,
Buffalo, New York 14260

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