Materials physics from first principles: from Feynman diagrams to solar cells

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During the past two decades, owing to the rapid development of electronic structure theory, high-performance computing, and software engineering, *ab initio* calculations based on density-functional theory (DFT) have emerged as a ubiquitous tool in materials research. The distinctive advantage of DFT techniques over phenomenological models is that they allow us to move from *descriptive* theories to *predictive* theories of materials and their properties [1]. As the popularity of DFT increases by the day, we are also beginning to appreciate more fully some of its fundamental limitations, for example the inability to reliably describe electronic and optical excitations. There is now mounting evidence that in order to achieve predictive power across the periodic table the most promising way forward is to power DFT with advanced Green's function techniques rooted in quantum field theory. In this talk I will discuss how we can now perform accurate calculations of electronic and optical excitations in semiconductors and insulators using field-theoretic approaches such as the GW method. In addition I will show how, after many decades of band structure calculations at zero temperature, field-theoretic approaches also provide us with a way to perform predictive electronic structure calculations at finite temperature [2,3]. I will illustrate the predictive power of these techniques by discussing recent work on the design of new organic-inorganic halide perovskites [4], the temperature-dependent optical properties of silicon [5], and the discovery of plasmonic polarons in semiconductors [6].

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