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Ab-initio electronic structure calculations of periodic systems in the presence of arbitrary magnetic fields[1] ALFREDO A. CORREA, EUNSEOK LEE, WEI CAI, Department of Mechanical Engineering, Stanford University, GIULIA GALLI, UC Davis — Ab initio electronic structure calculations in the presence of magnetic fields have been mainly performed for isolated systems, or, in the case of periodic systems, by adopting perturbative approaches. Building on a recent formulation of electronic structure calculations in the presence of magnetic fields [1,2], we will discuss calculations for periodic systems under arbitrary conditions, which include arbitrary (finite) magnetic field, arbitrary periodic cell shapes, and magnetic field spatial variations. Preliminary results based on a planewave numerical approach and local approximations to Density Functional Theory will be presented.[1] W.Cai, G.Galli, Phys. Rev. Lett. 92, 186402 (2004).[2] E. Lee, W. Cai, G. Galli, J. Comput. Phys. 226, 1310 (2007).

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