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First-principles approaches to electronic band structure of materials

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Electronic band structure is one of key properties of a material that has attracted ever-increasing interest in recent years thanks to tremendous efforts in solar-energy oriented photovoltaic and photocatalytic research. From the theoretical perspective, density functional theory in local density approximation or various generalized gradient approximations suffers from the well-known band gap problem[1]. Accurate theoretical prediction of electronic band structure of materials is therefore of great importance in both fundamental and applied research. Nowadays, the electronic band structure of the systems with weak electron correlations and relatively simple structures can be accurately described by Green’s function based many-body perturbation theory in the GW approach [2] and density functional theory in various hybrid functional approaches. On the other hand, there are still severe challenges for accurate theoretical prediction of electronic band structure of complex materials with complicated structure and/or compositions, and strongly correlated d/f-electron systems. In this work I will present our recent efforts to developing numerically accurate and efficient first-principles based theoretical approaches to electronic band structure of materials including numerically accurate GW approach in the linearized augmented planewaves (LAPW) framework [2], the perturbative modified Becke-Johnson potential [3] as a quick and pragmatic approach to electronic band structure of complex materials, and configurationally statistical averaging approach to electronic band structures of alloyed semiconductors.

[1] H. Jiang, Progress in Chemistry , 24, 910 (2012).
[2] H. Jiang, and P. Blaha, Phys. Rev. B, 93, 115203 (2016).
[3] H. Jiang, J. Chem. Phys. 138, 134115 (2013).