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Finite-basis correction applied to the optimized effective potential within the FLAPW method CHRISTOPH FRIEDRICH, MARKUS BETZINGER, STEFAN BLÜGEL, Institut fuer Festkoerperforschung and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — The optimized-effective-potential (OEP) method is a special technique to construct local exchange-correlation (xc) potentials from general orbital-dependent xc energy functionals for density-functional theory. Recently, we showed that particular care must be taken to construct local potentials within the all-electron full-potential augmented-plane-wave (FLAPW) approach. In fact, we found that the LAPW basis had to be converged to an accuracy that was far beyond that in calculations using conventional functionals, leading to a very high computational cost. This could be traced back to the convergence behavior of the density response function: only a highly converged basis lends the density enough flexibility to react adequately to changes of the potential. In this work we derive a numerical correction for the response function, which vanishes in the limit of an infinite, complete basis. It is constructed in the atomic spheres from the response of the basis functions themselves to changes of the potential. We show that such a *finite-basis correction* reduces the computational demand of OEP calculations considerably. We also discuss a similar correction scheme for *GW* calculations.

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