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Acceleration of the Convergence in *ab initio* Atomic Relaxations[1]
ZHENGJI ZHAO, LIN-WANG WANG, JUAN MEZA, LBNL — Atomic relaxations is often required to accurately describe the properties of nanosystems. In *ab initio* calculations, a common practice is to use a standard search algorithm, such as BFGS (Broyden-Fletcher-Goldfarb-Shanno) or CG (conjugate gradient) method, which starts the atomic relaxations without any knowledge of the Hessian matrix of the system. For example, the initial Hessian in BFGS method is often set to identity, and there is no preconditioning to CG method. One way to accelerate the convergence of the atomic relaxations is to estimate an approximate Hessian matrix of the system and then use it as the initial Hessian in BFGS method or a preconditioner in CG method. Previous attempts to obtain the approximated Hessian were focused on the use of classical force field models which rely on the existence of good parameters. Here, we present an alternative method to estimate the Hessian matrix of a nanosystem. First, we decompose the system into motifs which consist of a few atoms, then calculate the Hessian matrix elements on different motif types from *ab initio* calculations for small prototype systems. Then we generate the Hessian Matrix of the whole system by putting together these motif Hessians. We have applied our motif-based Hessian matrix in *ab initio* atomic relaxations in several bulk (with/without impurity) and quantum dot systems, and have found a speed up factor of 2 to 4 depending on the system size.

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