Convergence Acceleration of Relaxation-Separated Many-Body Expansion for Periodic Systems

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For exploration of configuration space in periodic systems, an efficient *ab initio* many-body expansion scheme is presented here. In the presented scheme, energy of a periodic system is separated into single point energy and relaxation energy as Fu *et al.* proposed[1], and each is approximated in terms of many-body expansion.

This approach was applied to spinel, layered, and olivine structures of cathode materials for sodium ion batteries. Convergence behavior of the expansion is investigated and weighting schemes for the expansion, both purely mathematical and semiempirical, are tested.

[1] Fu, G., Xu, X., Sautet, P. *Angew. Chem. Int. Ed.*, 51:1-6, 2012.