Multipole Expansion in Density-Functional Tight-Binding

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ABSTRACT

Density-functional tight-binding (DFTB) is an approximate method based on density functional theory (DFT), known for its computational efficiency, often being 2-3 orders of magnitude faster than traditional DFT. However, its accuracy in describing noncovalent interactions is limited due to its reliance on monopole-based charge densities. To address this limitation, we have developed an advanced version called multipole-extended DFTB (mDFTB), incorporating higher-order dipole and quadrupole interactions. Rigorous benchmarking against noncovalent interactions and proton transfer barriers demonstrates that the inclusion of multipole expansion significantly improves the accuracy of traditional DFTB. This advancement enhances the method's capability to model noncovalent interactions and proton transfers, making DFTB more versatile in computational chemistry.

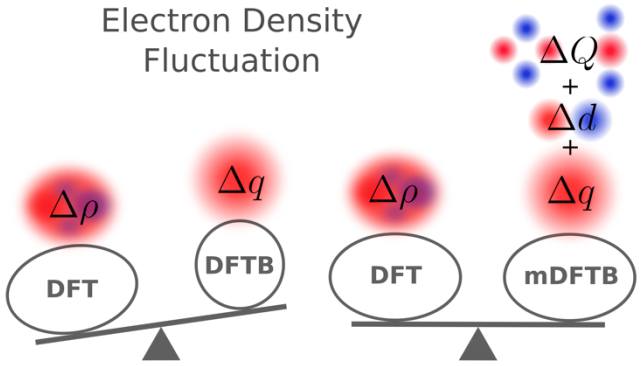

Figure 1: Graphical illustration showing effects of the multipole expansion in DFTB. [1]

References

[1] Vuong, V.-Q.; Aradi, B.; Niklasson, A. M. N.; Cui, Q.; Irle, S. Multipole Expansion of Atomic Electron Density Fluctuation Interactions in the Density-Functional Tight-Binding Method. *J. Chem. Theory Comput.* **2023**, *19*, 7592–7605.