DFTB: recent developments and remaining challenges

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Abstract

In this talk I'll provide an overview for the status and recent developments of the Density Functional Tight Binding (DFTB) model, especially those motivated by biophysical and solid/liquid interface applications. I'll discuss the treatment of non-covalent interactions with DFTB3. In particular, I'll present improvement of electronic polarization in DFTB3 and benchmark of the model using both gas phase and condensed phase examples. Next, I'll present progress and challenges for the development of DFTB3 for transition metal ions, which play important roles in many metalloenzymes. If time permits, I'll also comment on the use of DFTB3(/MM) as the low-level method to drive sampling in multi-level QM/MM free energy calculations.