

Structure Optimisation of Large Transition Metal Complexes with Extended Tight-Binding Methods

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Computer-aided theoretical investigations of large organometallic complexes are generally limited by the sheer size of real systems often consisting of hundreds to thousands of atoms. Accordingly, the development and evaluation of fast semiempirical quantum chemistry methods is indispensable. Here we report on the capability of the recently developed GFNn-xTB[1,2] methods, which are generally applicable for a large part of the periodic table including also lanthanoids[3] to perform full quantum mechanical geometry optimisation of large transition metal complexes and supramolecular organometallic structures. The results for a newly compiled benchmark set of 145 diverse closed-shell transition metal complexes including all transition metals up to Hg are presented. Additionally, the GFNn-xTB[1,2] methods are tested on established benchmark sets of organometallic reactions[4] and cross-checked for large and difficult show cases.

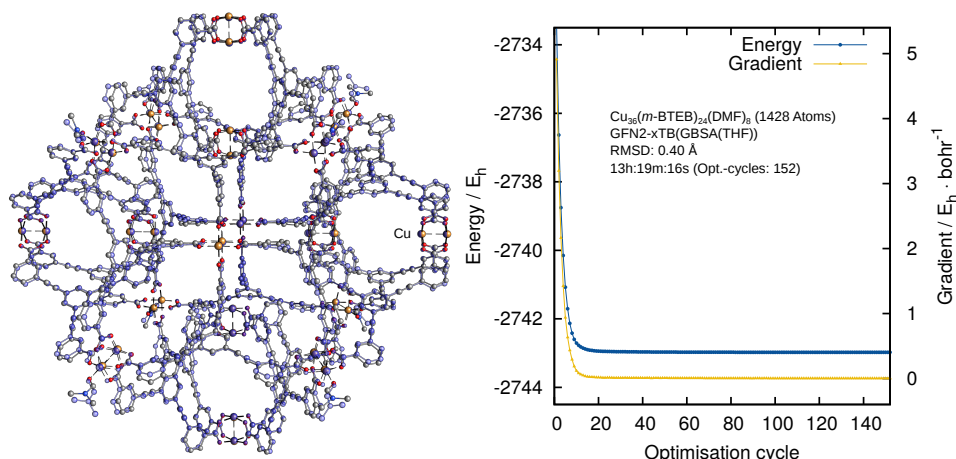


Figure 1: GFN2-xTB geometry optimisation of a large organometallic keplerate cage.[4]

References

1. S. Grimme, C. Bannwarth and P. Shushkov, *J. Chem. Theory Comput.* **13** (2017), 19892009.
2. C. Bannwarth, S. Ehlert and S. Grimme, *J. Chem. Theory Comput.* **15** (2019), 16521671.
3. M. Bursch, A. Hansen, S. Grimme, *Inorg. Chem.* **56** (2017), 1248512491.
4. M. Bursch, H. Neugebauer and S. Grimme, *Angew. Chem. Int. Ed.* (2019), DOI: 10.1002/anie.201904021.