

Metal Organic Frameworks (MOFs) are a very promising class of materials for various applications such as gas separation, detection and storage, shock absorbers, chemical catalysis and more. However, much research is still required before we can tap into the full potential of these materials, especially in the field of theoretical calculations. Although a lot has already been done, there is still much room for advancement. One of the main reasons, is that these MOF materials are computationally very challenging to simulate. Full ab initio calculations are very demanding and can only describe a limited time and length scale. Therefore, it is of crucial importance to have accurate force fields at hand to extend the theoretical simulations to larger time and length scales. Most of the force fields that are currently at hand are either not accurate enough or limited to one particular system. Therefore, in this work, we do not propose a new force field itself, but a methodology to quickly derive these force fields from ab initio calculations. By doing so, we combine the accuracy of system-tailored force fields with the general applicability of universal force fields. Although this methodology, called QuickFF, can in principle be applied to any system of choice, it was mainly developed to construct force fields for MOFs. Therefore, we will illustrate its performance here mainly for MOFs. The required input data consists of an ab initio calculation of the geometry and Hessian in equilibrium and if necessary a set of non-bonding parameters (charges and van der Waals parameters). The mathematical expression for the covalent energy is kept simple to ensure robustness and to avoid fitting deficiencies as much as possible. The proposed methodology is split into three steps: the first two steps address the strong correlations between parameters while the last step is a refinement of the model for higher accuracy. The resulting force fields are shown to accurately reproduce both the ab initio geometry and frequencies in equilibrium for a large set of small to medium-sized organic molecules and outperform well-known general force fields such as UFF and GAFF. Furthermore, it is illustrated that QuickFF can be used to easily derive accurate force fields for more complex systems such as MOFs. The methodology is implemented in a user-friendly Python code, which requires a minimum of input from ab initio calculations. As a result, accurate force fields for isolated molecules can easily be derived from ab initio calculations with only a minimal effort.