

# **Application of the Electronegativity Equalization Method for Evaluating the Charge Distribution in Porous Coordination Polymers**

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Electrostatic interactions play a dominant role in many modeling processes, when polar groups exist in the system under study. In computer simulation experiments, Density Functional Theory (DFT) calculations are performed to find the electron density of a molecule and, then, population analysis methods are applied to assign partial charges on the atoms. Despite that this process is computationally efficient for small molecules, it is prohibitive for large crystals like porous coordination polymers.

In this work, the computation of partial charges in porous coordination polymers is achieved by a combination of DFT and Electronegativity Equalization Method (EEM) calculations. In a first step, DFT and EEM computations on properly selected small crystal clusters are performed for the accurate extraction of input parameters to be used in the subsequent step of the EEM computations on the whole crystal structure, in order to take into consideration the chemical environment around each atom of the framework. This approach describes the proper use of DFT and EEM for the computation of partial charges in porous coordination polymers and brings out the method as a fast and computational efficient tool in atomistic experiments.