Atomic multipole moments for simulation of electrostatic potential and field in all siliceous zeolites

Larin A.V.[a)]*, Trubnikov D.N.[a)], Vercauteren D.P.[b)]

[a)] *Department of Chemistry, MSU, Moscow, GSP-2, 119992, Russia*
[b)] *University of Namur (FUNDP), Rue de Bruxelles 61, B-5000 Namur, Belgium*

Abstracts: A calibration method of atomic multipole moments (AMMs) is presented with respect to geometries of all siliceous zeolite models obtained from X-ray diffraction (XRD) methods. Mulliken atomic charges and AMMs are calculated for all siliceous types possessing small size elementary unit cells at the PDFT (PBE, B3LYP) with 88-31G*(Si)/8-411G*(O) and 66-21G*(Si)/8-411G*(O) basis sets and further used to fit several dependence functions *versus* the geometry variables for the Mulliken charges and *versus* special coordinates for the AMMs. The fitted parameters are introduced in CRYSTAL to propagate the electrostatic potential (EP) and electric field (EF) for all siliceous zeolites. The possibility of application of the point AMMs to classic simulation of physical adsorption is evaluated.