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Parameter Optimization for Charge Equilibration Method in Molecular Simulations EMERIC BOURASSEAU, JEAN-BERNARD MAILLET, CEA - DAM Ile de France - DPTA/PMC - France — In order to build a complete potential model to perform classical molecular dynamic simulations of dense liquids, a new optimization method is proposed to obtain transferable parameters for charge equilibration method. In order to make sure to obtain parameters which only describe coulombic interactions, the minimization of the error function is performed over data set constituted of pure electrostatic results taken from ab initio calculations. We first applied the new procedure to liquid HF systems. Some accurate ab initio calculations have been performed using the VASP code to completely characterize dense liquid of HF (Maillet et al., accepted to Phys. Rev. B, 2005). Electrostatic potential grids have been calculated for several configurations taken from those simulations, and optimization of parameters used in charge equilibration method has been performed on some points of those grids. The optimized parameters (the electronegativity χ and the Slater orbital exponent ζ for H and F atoms) appear able to reproduce the variations of the electrostatic potential calculated from ab initio method for different thermodynamic conditions. It is concluded that the proposed method is general, precise and efficient to obtain transferable and realistic parameters.

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