DEVELOPMENT OF TRANSFERABLE INTERACTION MODELS FOR WATER FROM FIRST PRINCIPLES: WATER CLUSTERS, LIQUID WATER AND SEVERAL FORMS OF ICE

SOTIRIS S. XANTHEAS, CHRISTIAN J. BURNHAM, *Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 906 Battelle Boulevard, PO Box 999, MS K8-91, Richland, WA 99352, USA*.

We present the development of a flexible, all-atom polarizable empirical model for water that is parameterized using the results of first principles electronic structure calculations for water clusters. The model employs smeared charges and dipole sites and it is based on Thole's method for describing molecular polarizabilities. It is fitted to "chemically important" parts of the water dimer potential energy surface obtained from highly accurate electronic structure calculations. It reproduces the temperature dependence of the second virial coefficient over the temperature range 423-773 K, the total binding energies of water clusters n=2-8 to within an accuracy of 1% or better with respect to the MP2/CBS (complete basis set) estimates. Results of liquid properties such as the diffusion constant and radial distribution functions as well as lattice parameters and relative energetics for several forms of ice such as Ih, II and XI obtained with the model will also be presente! d.