A Dynamic Charge Potential for Water

KRISHNA MURALIDHARAN, University of Florida, SUSAN ATLAS, University of New Mexico, STEVE VALONE, Los Alamos National Labs, KEITH RUNGE, University of Florida — We present a new ab initio based interatomic potential for water clusters and liquid water capable of accounting for electronic induction through hydrogen bonding and non-bonding interactions. Though the functional form of the potential is similar to embedded atom method (EAM) formulations, an important difference lies in the fact that the atomic electron densities are environment dependent. This study modifies EAM methods to describe systems, like water, where the role of induction is vital.