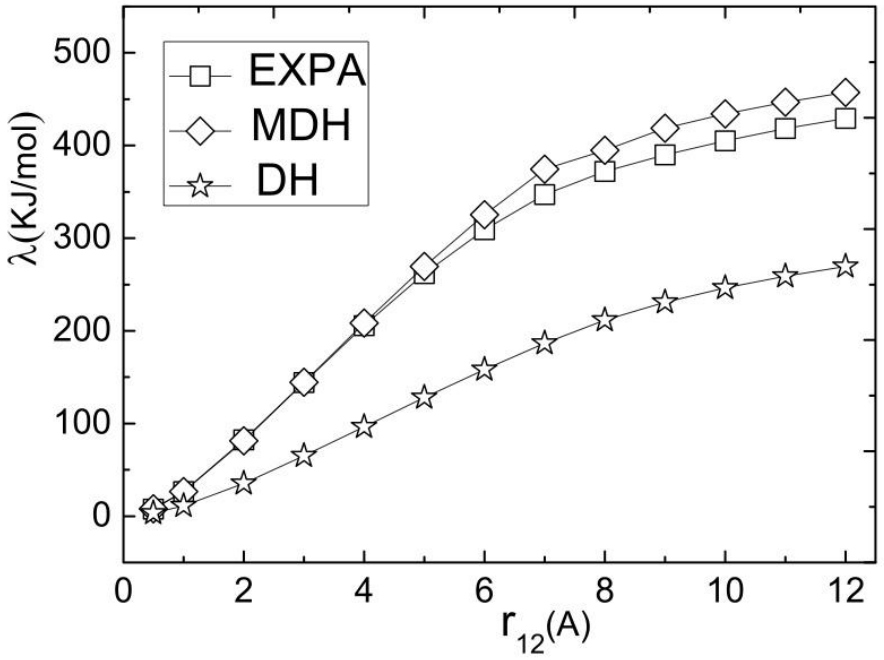
Reorganization energy of electron transfer process in ionic fluids : a molecular Debye-Hückel approach

Tiejun Xiao and Xueyu Song



Dependence of reorganization energy λ on the site distance r_{12} of a diatomic model of electron transfer reaction from molecular simulations(EXPA) (square), our MDH theory (diamond), and conventional DH theory(star). The lines are guides to the eye.