A GLOBAL MODEL FOR LONG-RANGE INTERACTION ‘DAMPING FUNCTIONS’

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In recent years, ‘damping functions’, which characterize the weakening of inverse-power-sum long-range interatomic interaction energies with increasing electron overlap, have become an increasing important component of models for diatomic molecule interaction potentials. However, a key feature of models for damping functions, their portability, has received little scrutiny. The present work set out to examine all available ab initio induction and dispersion damping function data and to attempt to devise a ‘global’ scheme for diatomic molecule damping functions. It appears that while neutral (H, He, Li, and Ne, homonuclear and mixed) and anion (H\(^+\) with H, He and Li) species obey (approximately) one common rule, proton plus neutral (H\(^+\) with H, He and Li) and non-proton-cation plus neutral systems (He\(^+\) and Li\(^+\) with H, He and Li), must each be treated separately. However, for all three cases, a version of the Douketis-Scoles-Thakkar\(^\text{c}\) (ionization potential)\(^\text{power} \) factor is a key scaling parameter.