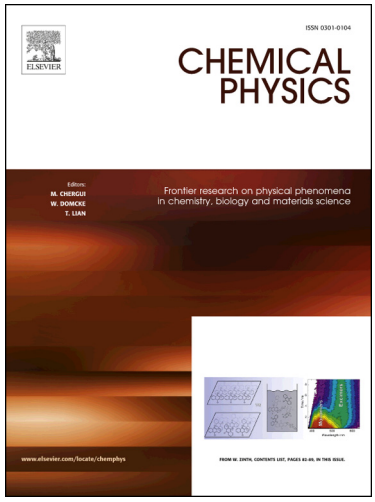

New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmitters' amino group acidity

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New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmitters' amino group acidity

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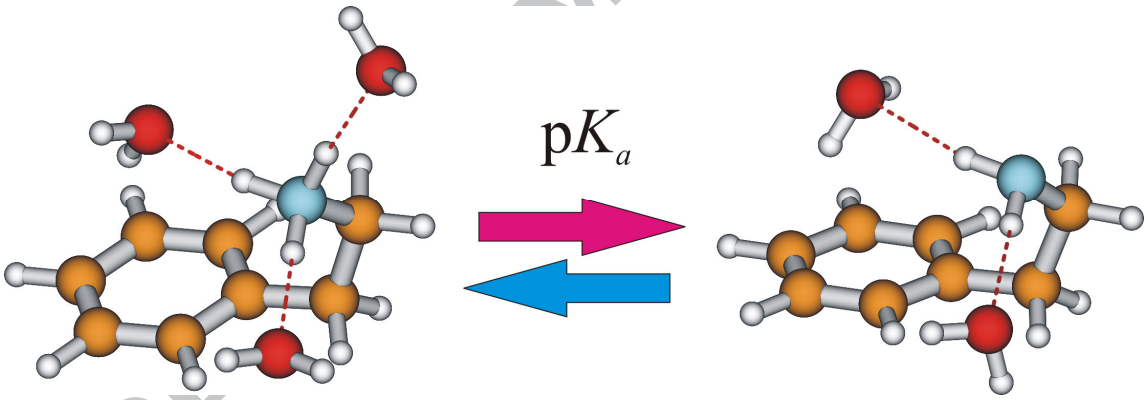
Hybrid cluster-continuum model.

pKa values calculations.

Primary amines.

Molecular dynamics simulations.



Abstract: Acid dissociation constant is a quantitative measure of chemical species ability to donate a proton to water molecule and plays important role in aqueous chemistry. Many computational strategies were conceived in order to properly address an acid dissociation equilibrium. In this work, we present new economical cluster-continuum method based on the density functional theory for the accurate calculation of pK_a values. By analysing hydration properties of neutral and protonated 2-phenylethylamine sampled in the first principle molecular dynamics simulations, we were able to find key interactions between water