

Dynamic Protonation and Deprotonation Reactions in
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Protons have been considered as potential charge carriers in constructed nanoscale semiconductors. They are attractive because, in the condensed state, they can move from one protonatable molecule to another with high mobility. Furthermore, they have been implicated as the triggers that modulate gating mechanisms in biological ion channels, a function that could be harnessed to actuate nanoscale devices, as well. In an effort to model proton motion, we have applied ab initio methods to study dynamic protonation/deprotonation in the amino acid, glycine. While a neutral form of glycine is most stable in the gas phase, proton transport occurs in liquid water to produce a zwitterion molecule. We will report on our simulations of the protonation reaction, our estimates of the relative thermodynamic stabilities of the different forms of glycine, as well as our estimates of activation barriers for interconversions between these forms.