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Enabling proton transfer in classical simulations

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An important limitation of mainstream classical molecular dynamics simulations is the inability to make or break chemical bonds. This limitation is especially restrictive in regard to protons and hinders our ability to model processes involving proton transfer. Existing approaches for allowing proton transfer in the context of classical mechanics are still cumbersome and have not achieved widespread use and routine status. Here we consider a simple combination of molecular dynamics with periodic stochastic proton hops. To ensure computational efficiency, we propose a non-Boltzmann acceptance criterion that is heuristically adjusted to maintain the correct or desirable thermodynamic equilibria between different protonation states and proton transfer rates. Parameters are proposed for hydronium, hydroxide, Asp, Glu, and His. The algorithm is implemented in the program CHARMM and tested on proton and hydroxide diffusion in bulk water and carbon nanotubes and proton conductance in the gramicidin A channel.