Developing improved MD and QMMM codes for modeling enzymes essential to biomass liquid fuel production

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Understanding the mechanisms and improving the efficiency of the hydrolysis of cellulose for the production of liquid biofuels is critical for our energy future. The mechanism of action of cellulose-degrading enzymes can be illuminated through a multidisciplinary collaboration that uses molecular dynamics (MD) and hybrid quantum mechanics molecular mechanics (QMMM) simulations. This paper details efforts to improve the efficiency of MD codes, as well as the addition of PM6 semiemperical hybrid QMMM functionality to such codes. Our efforts expand the capabilities of MD codes to allow simulations of enzymes and substrates on petascale computational facilities.