A Case Study in Performance Evaluation of Density Functional Tight Binding Method in Two Layer ONIOM Method

Tzvetelin D. Iordanov

Department of Chemistry, Georgia Southwestern State University,
800 Georgia Southwestern State University Drive, Americus, GA 31709

A performance evaluation of Density Functional Tight Binding (DFTB) in the two-layer ONIOM method is presented in an effort to estimate DFTB effectiveness as an inexpensive low level quantum mechanical layer. Ground state geometries, geometry error, S-values, and energy error for: $(H_2O)_x(MeOH)_y$, $[(\eta^5\text{-}C_5Me_nH_{5-n})_2Ti]_2(\mu_2,\eta^2,\eta^2\text{-}N_2)$, n=4, and complexes of Cu^+ with tyrosine, were compared to target calculations at B3LYP level of theory for all three of the systems and second order Moller-Plesset (MP2) target level of theory for the first two systems. The calculated root mean squared errors (RMS) of the ONIOM optimized geometries relative to the target are found to be small. The DFTB level of theory was unable to reproduce the target geometry structure for one of the isomers of tyrosine-Cu^+ complex, while the ONIOM combinations were able to reproduce all target structures. The absolute value of the geometry error was determined to be smaller then the corresponding energy error except for the $(H_2O)_x(MeOH)_y$ system at the ONIOM(MP2/6-31G(d,p):DFTB) level of theory. The S-values were relatively small and close in value contributing to relatively small energy errors. Both method combinations ONIOM(MP2:DFTB) and ONIOM(DFT:DFTB) show similar performance compared to the corresponding target level of theory.