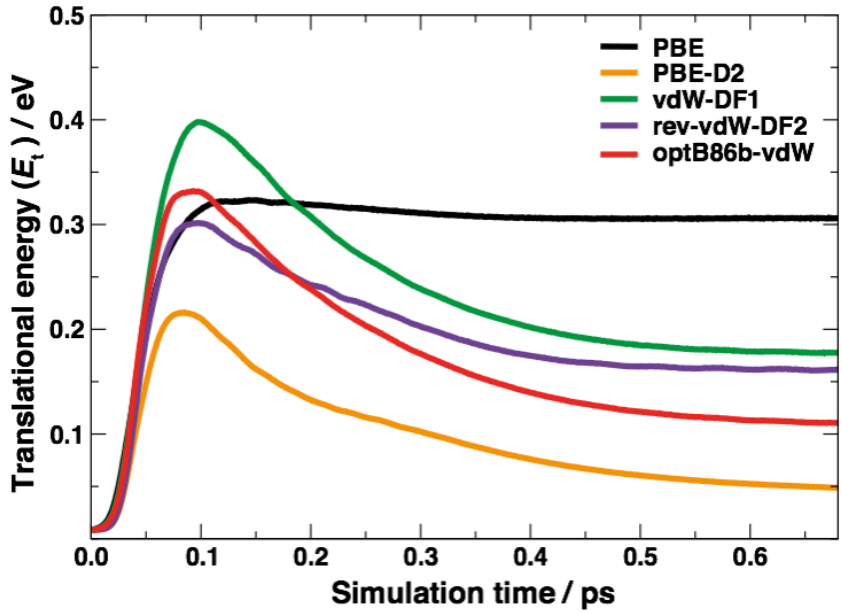


**Figure 1.** Time evolution of the translational energy of desorbed $CO_2$ from formate decomposition calculated using PBE, PBE-D2, and vdW-DFs.

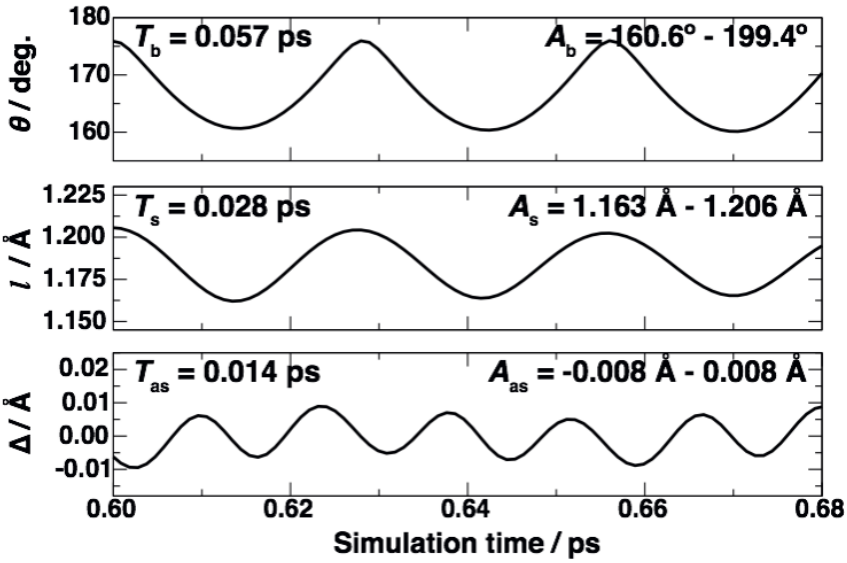


**Figure 2.** Time evolution of $CO_2$ bond angle ($\theta$), the C–O bod length ($l$), and the difference between two C–O bond lengths ($\Delta$) based on molecular dynamics trajectory calculated using optB86b-vdW functional. The period ($T$) and amplitude ($A$) of each geometry data are shown in each panel.