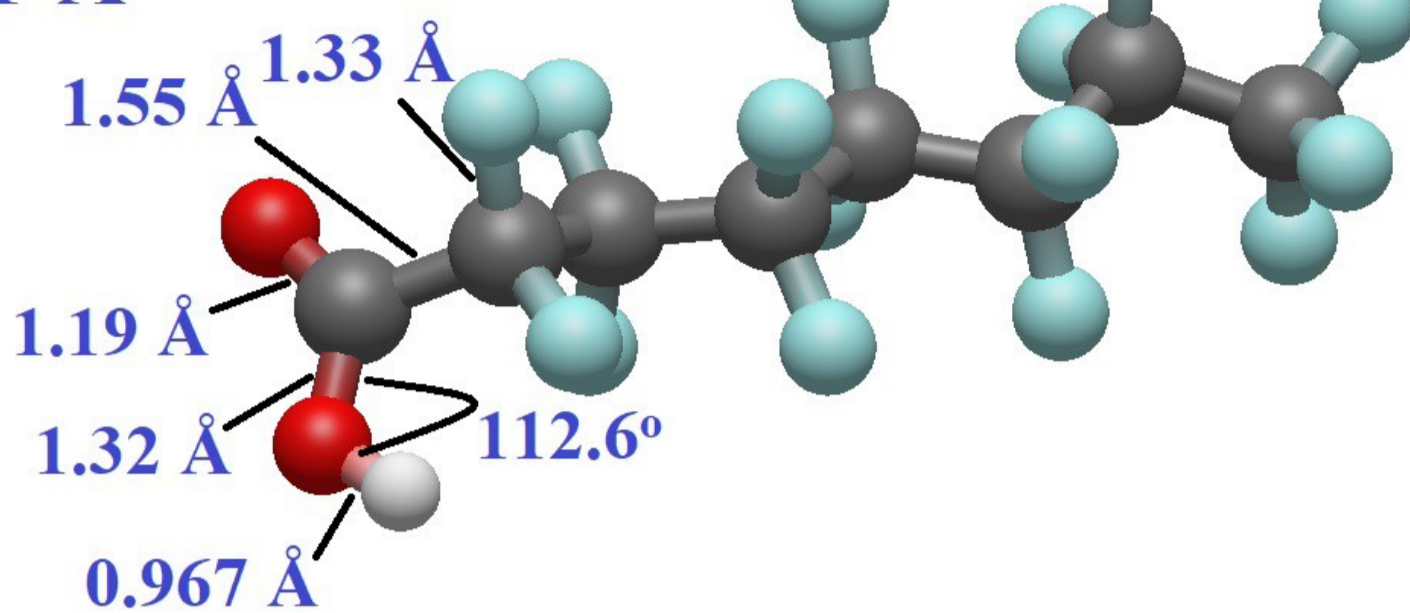


PFOA

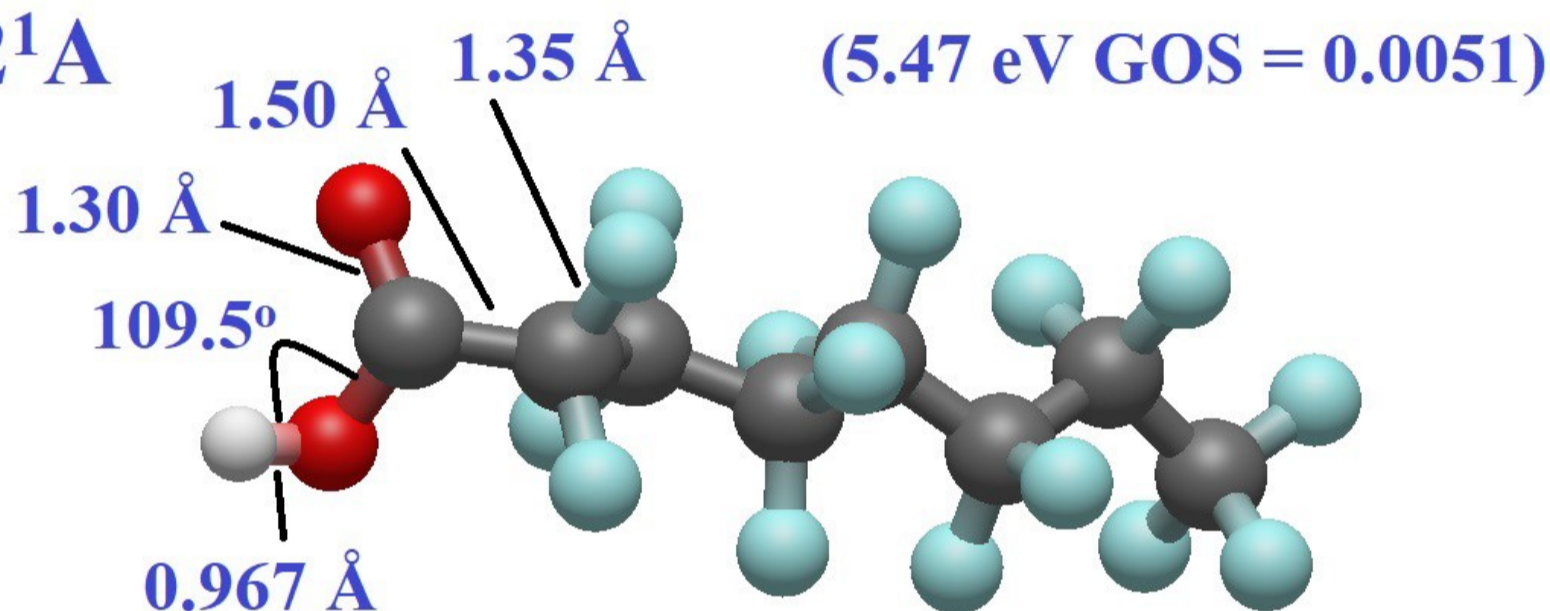
TD-DFT/M06-2X/6-311+G(2d,2p)

(protonated)

1¹A

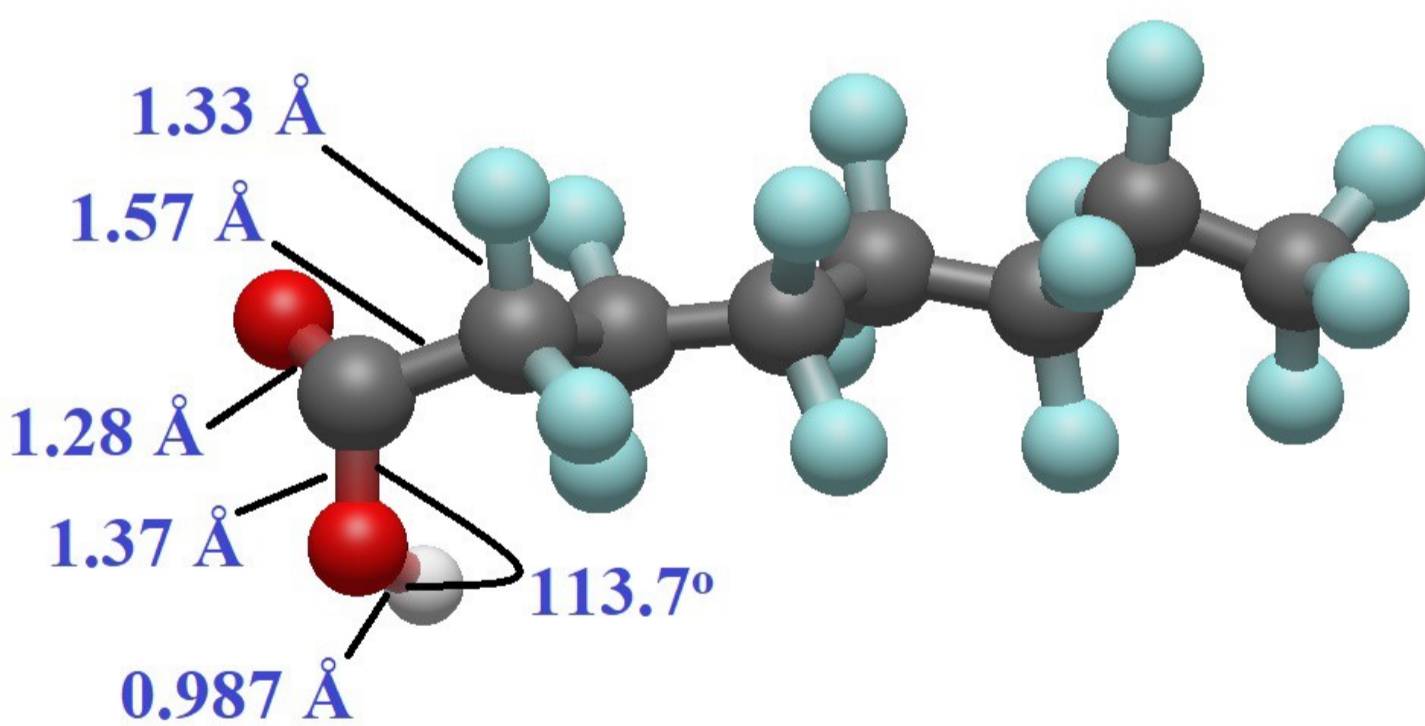


2¹A



3¹A

(8.10 eV GOS = 0.1571)



LUMO

