Density Functional Reactivity Theory and its Applications in Solar Energy Research

Shubin Liu

Research Computing Center, University of North Carolina, Chapel Hill, NC 27599-3420

Density functional reactivity theory (DFRT) is the chemical reactivity theory of density functional theory (DFT), first proposed and developed by R.G. Parr and coworkers of UNC-CH in 1980s. In this contribution, recent theoretical developments of DFRT by the present author are outlined, including quantifying electrophilicity and steric effect. Approaches as well as applications to quickly and reliably predict molecular acidity (pKa values) and the proton-coupled electron transfer (PCET) reaction mechanism using reactivity descriptors from DFRT for solar energy related systems are also presented. Put together, these novel approaches provide new opportunities for the design of next generation catalysts for H_2O oxidation and CO_2 reduction reactions.

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