

## Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error

In recent years, the physical interpretation of occupied Kohn-Sham eigenvalues as vertical ionization potentials has been proposed, based on several formal and numerical arguments. Similarly, the performance of density functional approximations (DFAs) for fractionally charged systems has been extensively studied as a measure of one- and many-electron self-interaction errors (MSIE). These (in principle unrelated) perspectives suggest that new functionals should aim to produce accurate orbital eigenvalues and/or exact fractional charge behavior, to remedy long-standing pathologies of DFAs. In this contribution, we show that IP-optimized functionals (the CAM-QTP family) display reduced self-interaction errors in a variety of tests. Conversely, the MSIE-optimized rCAM-B3LYP functional also displays accurate orbital eigenvalues. This suggests that the conditions required to fulfill Bartlett's IP-theorem are closely related to the conditions required to reduce MSIE. Additionally, it is shown that the CAM-QTP and rCAM-B3LYP functionals show improved dissociation limits, fundamental gaps and thermochemical accuracy compared to their parent functional CAM-B3LYP.