Benchmarking ionization potentials from the simple pCCD model

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The electron-detachment energy is measured by its ionization potential (IP). As a result, it is a fundamental observable and important molecular electronic signature for photoelectron spectroscopy investigation of chemical substances. A precise theoretical prediction of this feature is essential for virtual organic optoelectronic systems like transistors, solar cells, and LEDs. In this work, we benchmark the performance of the recently presented IP variant of the equation-of-motion pair coupled cluster doubles (IP-EOM-pCCD) model in predicting IPs. Specifically, the anticipated IPs are compared to experiments and higher-order coupled cluster theories based on statistically assessing roughly 200 electron-detached states of 41 molecules. Our study will highlight the accuracy and reliability of the inexpensive and straightforward IP-EOM-pCCD model compared to more elaborate approaches.