

Abstract Submitted
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The quantum defect: the true measure of TDDFT results for atoms META VAN FAASSEN, KIERON BURKE, Department of Chemistry and Chemical Biology, Rutgers University — We apply quantum defect theory to (time-dependent) density-functional calculations of Rydberg series for some closed shell atoms. We will compare several potentials by considering the quantum defect instead of the excitation energies. The quantum defect has the property of amplifying errors, allowing us to show that results that seem accurate from tables of excitation energies are not always so, especially for larger values of the principle quantum number n . In this way the quantum defect provides the appropriate tool for comparing time-dependent density-functional results for atoms.

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