Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Rydberg transitions from the local density approximation[1] KIERON BURKE, Rutgers University, ADAM WASSERMAN, Harvard University — Using quantum defect theory, we show how to extract accurate Rydberg transitions (both frequencies[1] and oscillator strengths[2]) from density functional calculations using the local density approximation, despite the short-ranged potential. For the case of He and Ne, the asymptotic quantum defects predicted by the calculations are in less than 5% error, yielding transition frequency errors of less than 0.1 eV.

[1]Rydberg transition frequencies from the Local Density Approximation A. Wasserman and K. Burke, Phys. Rev. Lett. 95, 163006 (2005).
[2]Accurate Rydberg Excitations from Local Density Approximation A. Wasserman, N.T. Maitra, and K. Burke, Phys. Rev. Lett. 91, 263001 (2003).

[1]Work supported by NSF CHE-0355405

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Date submitted: 23 Nov 2005 Electronic form version 1.4