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Self-Consistent Random Phase Approximation DANIEL ROHR, Rice University, Houston, TX, MARIA HELLGREN, E.K.U. GROSS, Max-Planck-Institute, Halle, Germany — We report self-consistent Random Phase Approximation (RPA) calculations within the Density Functional Theory. The calculations are performed by the direct minimization scheme for the optimized effective potential method developed by Yang et al. [1]. We show results for the dissociation curve of H_2^+, H_2 and LiH with the RPA, where the exchange correlation kernel has been set to zero. For H_2^+ and H_2 we also show results for RPAX, where the exact exchange kernel has been included. The RPA, in general, over-correlates. At intermediate distances a maximum is obtained that lies above the exact energy. This is known from non-self-consistent calculations and is still present in the self-consistent results. The RPAX energies are higher than the RPA energies. At equilibrium distance they accurately reproduce the exact total energy. In the dissociation limit they improve upon RPA, but are still too low. For H_2^+ the RPAX correlation energy is zero. Consequently, RPAX gives the exact dissociation curve. We also present the local potentials. They indicate that a peak at the bond midpoint builds up with increasing bond distance. This is expected for the exact KS potential.

[1] W. Yang, and Q. Wu, *Phys. Rev. Lett.*, **89**, 143002 (2002)

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