

Faddeev Random Phase Approximation for Molecules

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The many body Green's function is an adequate tool to study the ground-state energy and ionization energies of molecules. The Faddeev Random Phase Approximation (FRPA)[1] makes use of Faddeev-equations to couple two-particle - one-hole (2p1h) and two-hole - one-particle (2h1p) excitations to the single-particle spectrum. Solving these equations implies an infinite partial summation of the perturbation expansion of the self-energy. This method goes beyond the ADC(3)[2] approximation by treating both the particle-hole and particle-particle interactions at the RPA level. We present the results of our calculations for some diatomic molecules.

References

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- [2] J. Schirmer, L. S. Cederbaum, O. Walter, Phys. Rev. A **28**, 1237 (1983).