

Abstract Submitted
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First-principles calculation of optical excitations in azobenzene ($C_{12}H_{10}N_2$)¹ MURILO L. TIAGO, JAMES R. CHELIKOWSKY, University of Minnesota — The photo-isomerization of azobenzene, $C_{12}H_{10}N_2$, is a long-standing theoretical problem which has been studied recently with time-dependent density-functional theory (TDDFT) and methods based on configuration interaction (CI). The central problem resides in determining the behavior of optically excited states in the molecule as its geometric configuration evolves from cis to trans-azobenzene and vice-versa. In order to get an accurate description of optical excitations in the system, we use Green's function methods based on the GW approximation and Bethe-Salpeter Equation (BSE). In this implementation, we take advantage of the finite extent of electronic wave-functions, which reduces significantly the numerical cost, without compromising accuracy. We discuss the dependence of excitation energies with respect to the CNNC dihedral angle, as the molecule undergoes isomerization. Results obtained with the BSE and TDDFT methods are compared.

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