

## **time-dependent density functional theory**

**Acronym:** TD-DFT

Methods for computing accurate excitation energies at a low computational cost in large molecular species within the time-dependent scheme and the density functional theory. It is the only available DFT-based method for computing electronic excitation energies.

**Source:**

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 433