

Abstract Submitted
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TDDFT and qualitative properties of excited states: three illustrative applications using DMol³ BERNARD DELLEY, Paul Scherrer Institut, CMT — Three applications of DMol³ TDDFT [1] are presented to show possible new frontiers in each case. First, excitations involving multiplet structure for the example of the Ti⁴⁺ ion are discussed, showing that atomic multiplet splitting is fully exhibited within TDDFT. This approach to multiplets exhibits notable similarities and also notable differences with a first principles based Condon-Shortley-Cowan multiplet theory. Second, UV-VIS spectra of benzene and derivative molecules are discussed by comparing experimental log plots of molar extinction with a TDDFT results completed by the Gaussian envelope model for the vibrational progression. The envelope model provides a natural scale for comparing TDDFT excitations with measured absorption spectra. In the third example, excited states of (Fe(CN)₅NO)⁻² are studied along the reaction coordinate connecting the long lived metastable states that can be produced by optical excitation.

[1] B. Delley, J. Phys. Cond. Mat. 22, 384208, 2010.

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