TDDFT and qualitative properties of excited states: three illustrative applications using DMol$^3$ BERNARD DELLEY, Paul Scherrer Institut, CMT — Three applications of DMol$^3$ TDDFT [1] are presented to show possible new frontiers in each case. First, excitations involving multiplet structure for the example of the Ti$^{4+}$ 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)$_5$NO)$^{-2}$ are studied along the reaction coordinate connecting the long lived metastable states that can be produced by optical excitation.