Supporting Information for Beyond the Coulson-Fischer point: Characterizing single excitation CI and TDDFT for excited states in single bond dissociations

Diptarka Hait,¹,a) Adam Rettig,¹,a) and Martin Head-Gordon¹,²,b)

¹) Kenneth S. Pitzer Center for Theoretical Chemistry, Department of Chemistry, University of California, Berkeley, California 94720, USA

²) Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

a) These authors contributed equally to this work.

b) Electronic mail: mhg@cchem.berkeley.edu
FIG. 1: $M_S = 0$ TDDFT and TDDFT/TDA excited states predicted for NH$_3$/aug-cc-pVTZ.
FIG. 2: $M_S = 0$ TDDFT and TDDFT/TDA excited states predicted for $C_2H_6$/aug-cc-pVDZ.
FIG. 3: $M_S = 0$ TDDFT and TDDFT/TDA excited states predicted for LiH/aug-cc-pVTZ. Note that the PBE surfaces have an additional kink around 5Å of separation, which probably originates from the significant delocalization error driven CT contamination in the UPBE ground state.
FIG. 4: $M_S = 1$ TDDFT/TDA excited states predicted for NH$_3$/aug-cc-pVTZ (along with the corresponding UKS ground state).

FIG. 5: $M_S = 1$ TDDFT/TDA excited states predicted for C$_2$H$_6$/aug-cc-pVDZ (along with the corresponding UKS ground state).
FIG. 6: $M_S = 1$ TDDFT/TDA excited states predicted for LiH/aug-cc-pVTZ (along with the corresponding UKS ground state). Note that the PBE surfaces have a discontinuity around 5Å of separation, which probably originates from the significant delocalization error driven CT contamination in the UPBE ground state.