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

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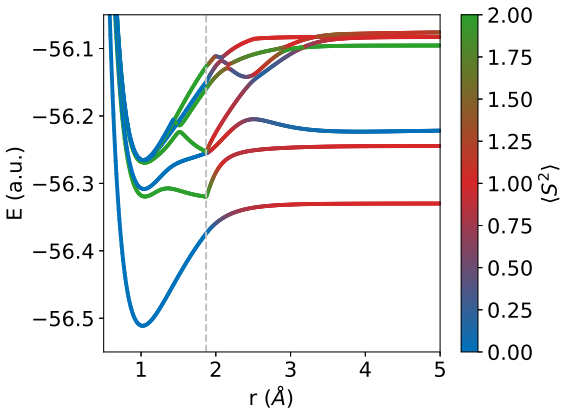
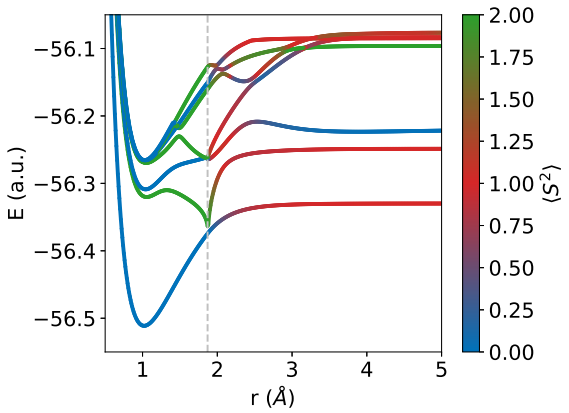
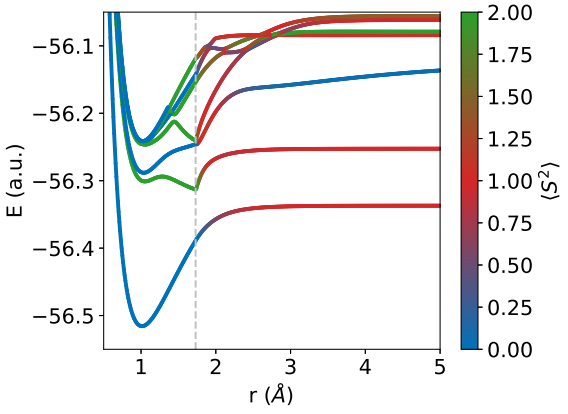


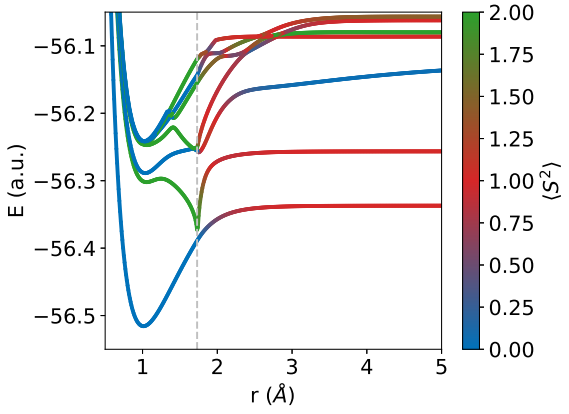
(a) PBE/TDA



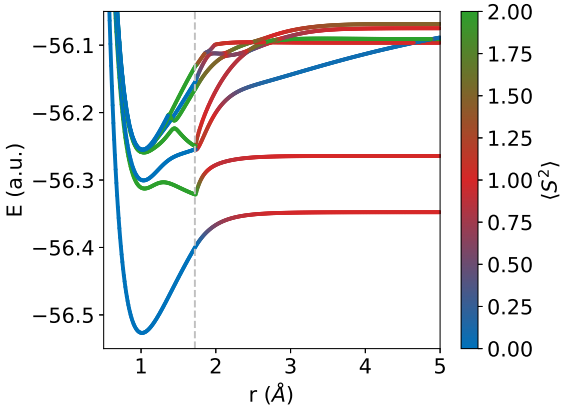
(b) PBE/TDDFT



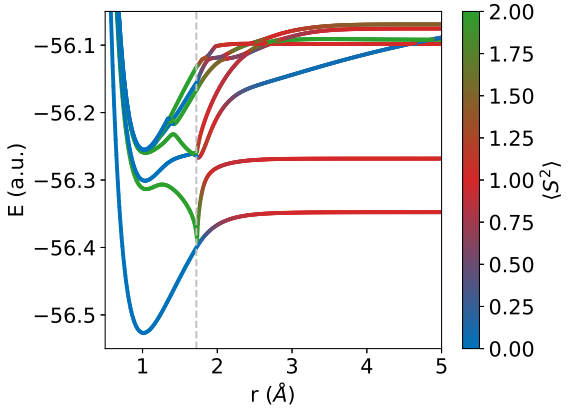
(c) PBE0/TDA



(d) PBE0/TDDFT

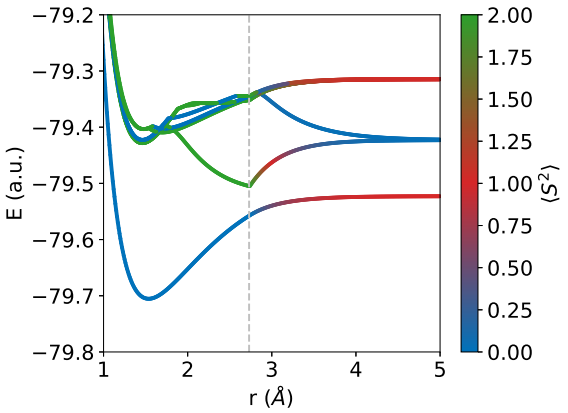


(e) LRC-ωPBEh/TDA

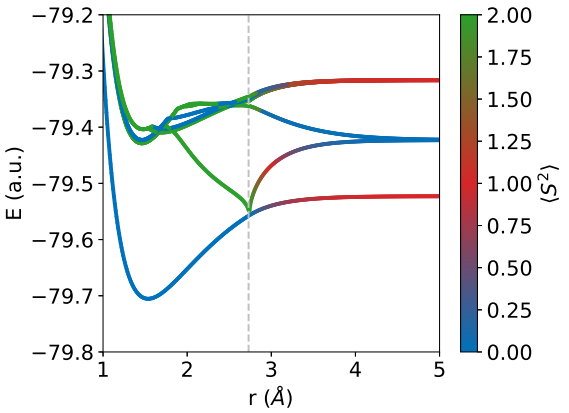


(f) LRC-ωPBEh/TDDFT

FIG. 1: $M_S = 0$ TDDFT and TDDFT/TDA excited states predicted for NH_3/aug-cc-pVTZ.



(a) PBE/TDA



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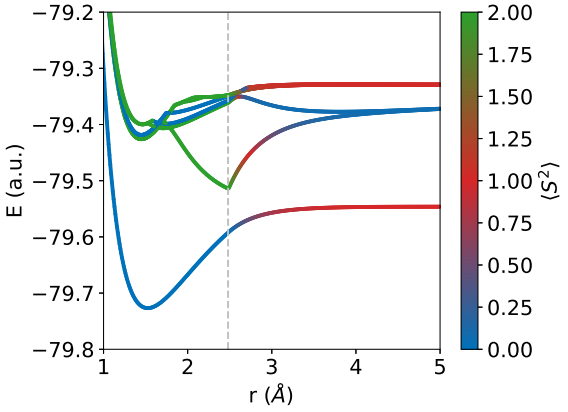
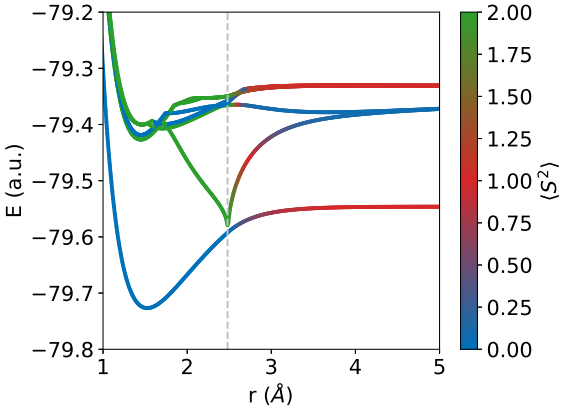


(c) PBE0/TDA



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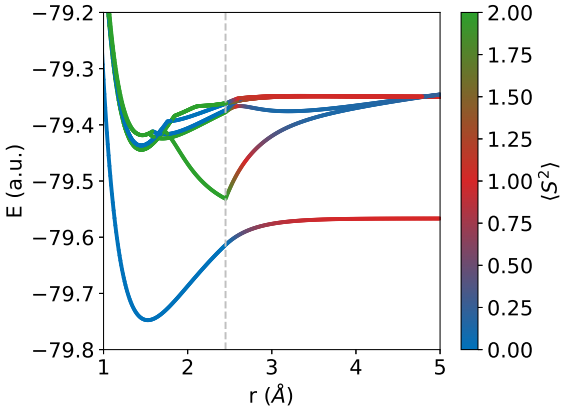
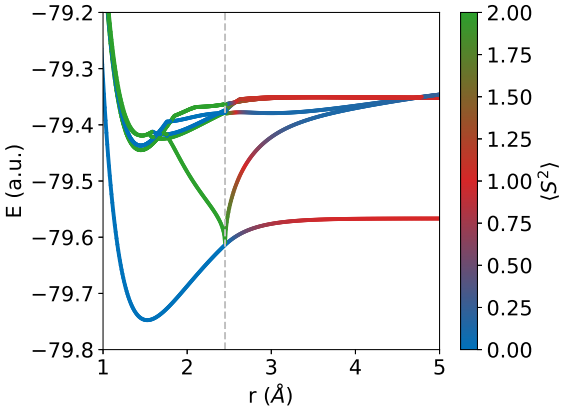
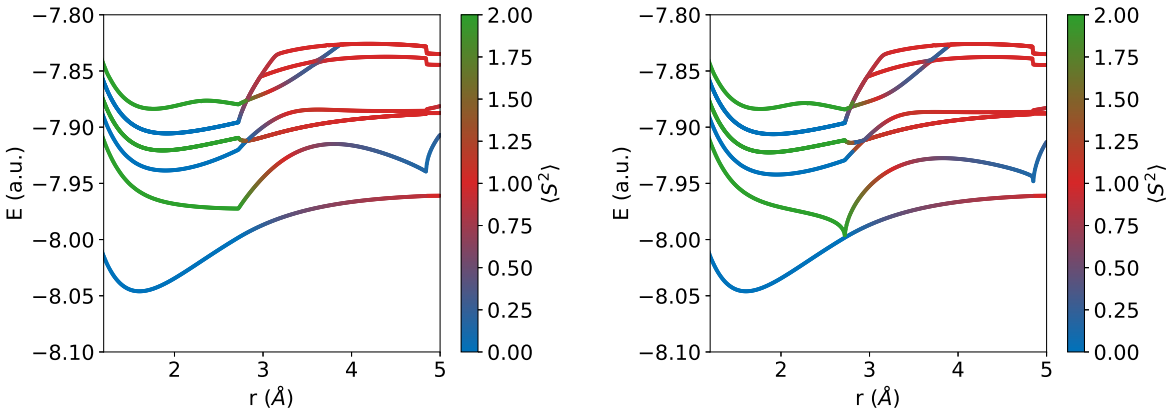


(e) LRC-ωPBEh/TDA



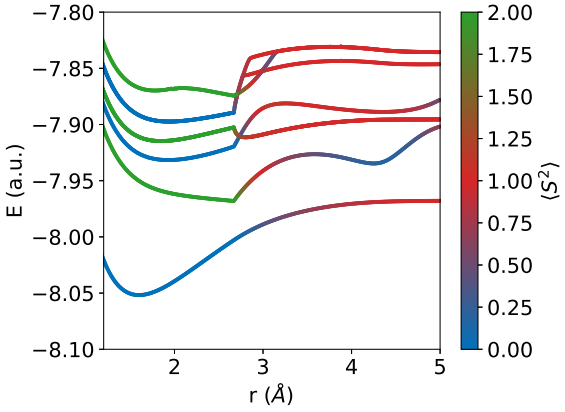
(f) LRC-ωPBEh/TDDFT

FIG. 2: $M_S = 0$ TDDFT and TDDFT/TDA excited states predicted for C_2H_6/aug-cc-pVDZ.



(a) PBE/TDA

(b) PBE/TDDFT



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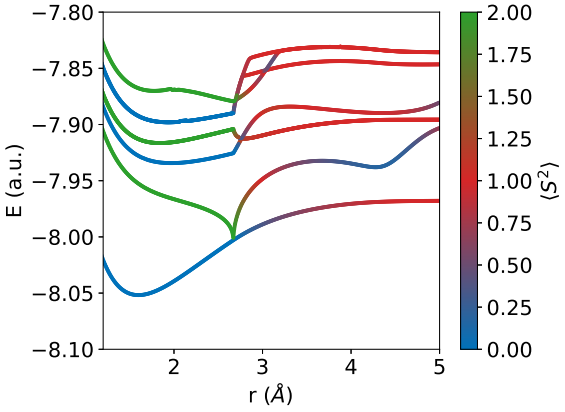

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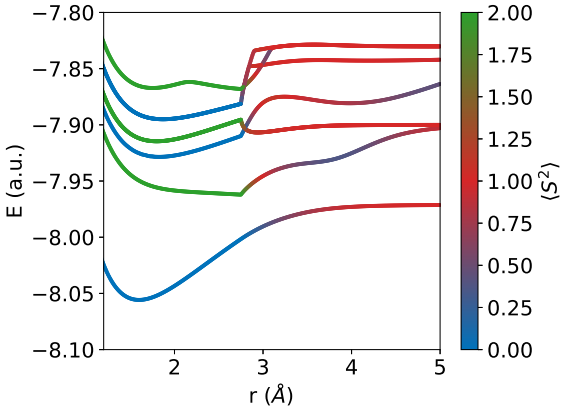
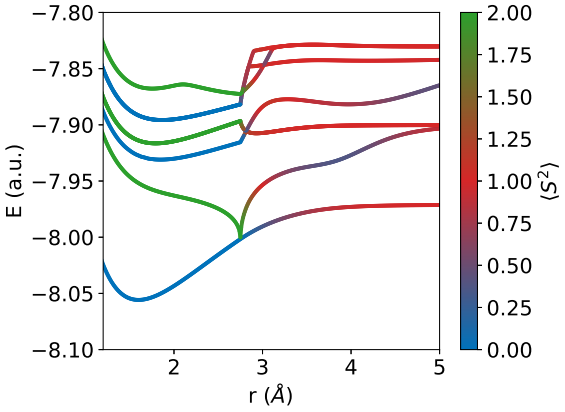
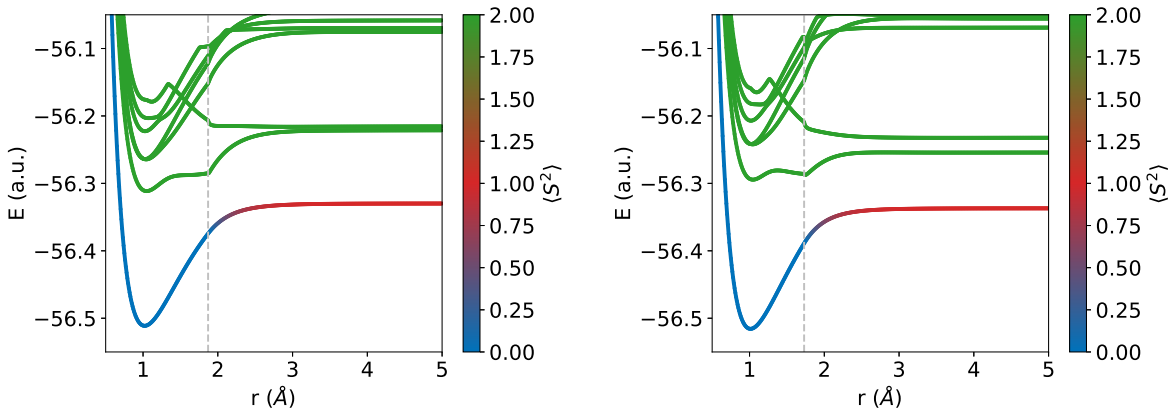


(e) LRC-ωPBEh/TDA



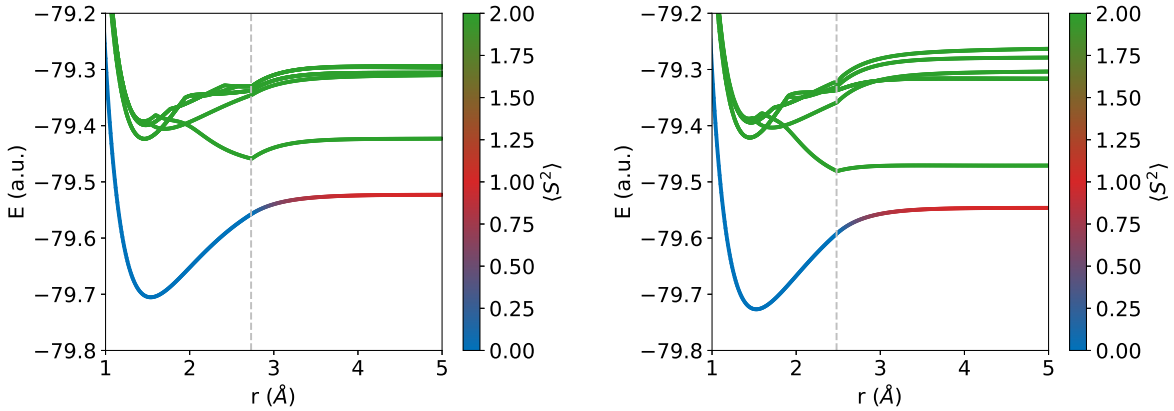
(f) LRC-ωPBEh/TDDFT

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.



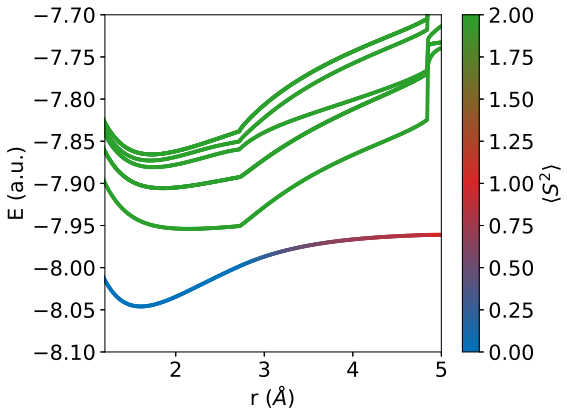
(a) PBE/TDA (b) PBE0/TDA

FIG. 4: $M_S = 1$ TDDFT/TDA excited states predicted for NH_3/aug-cc-pVTZ (along with the corresponding UKS ground state).

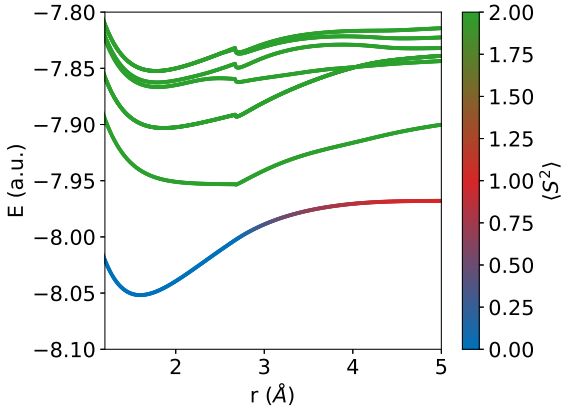


(a) PBE/TDA (b) PBE0/TDA

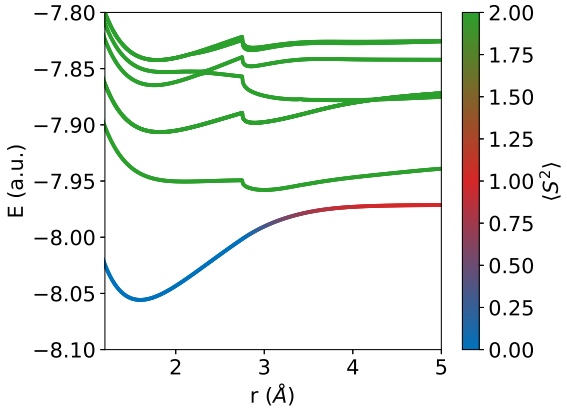
FIG. 5: $M_S = 1$ TDDFT/TDA excited states predicted for C_2H_6/aug-cc-pVDZ (along with the corresponding UKS ground state).



(a) PBE/TDA



(b) PBE0/TDA



(c) LRC-ωPBEh/TDA

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.