STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 77 (2021)

Supporting information for article:

X-ray restrained extremely localized molecular orbitals for the embedding of quantum mechanical calculations

Giovanni Macetti, Piero Macchi and Alessandro Genoni

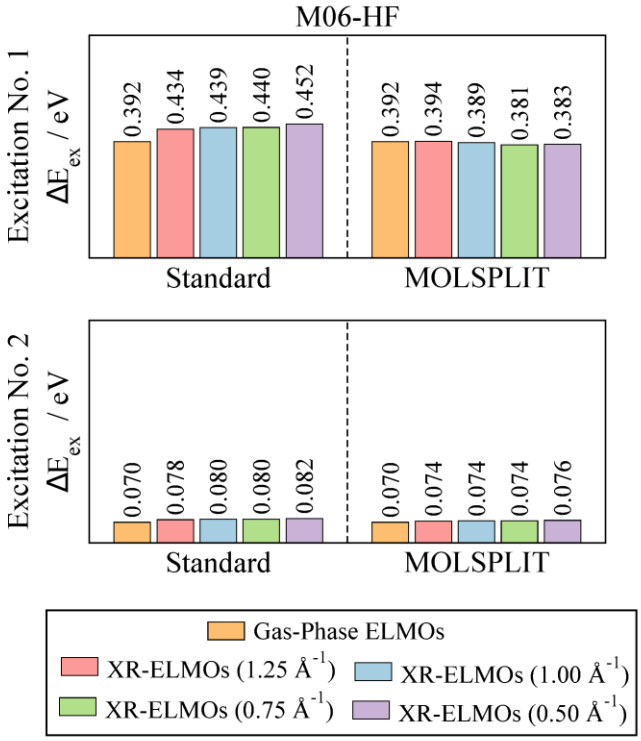

Figure S1 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from EOM-CCSD/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of X-ray datasets associated with periodic M06-HF densities (standard and MOLSPLIT) and characterized by different maximal resolutions (1.25 Å^{-1}, 1.00 Å^{-1}, 0.75 Å^{-1} and 0.50 Å^{-1}).

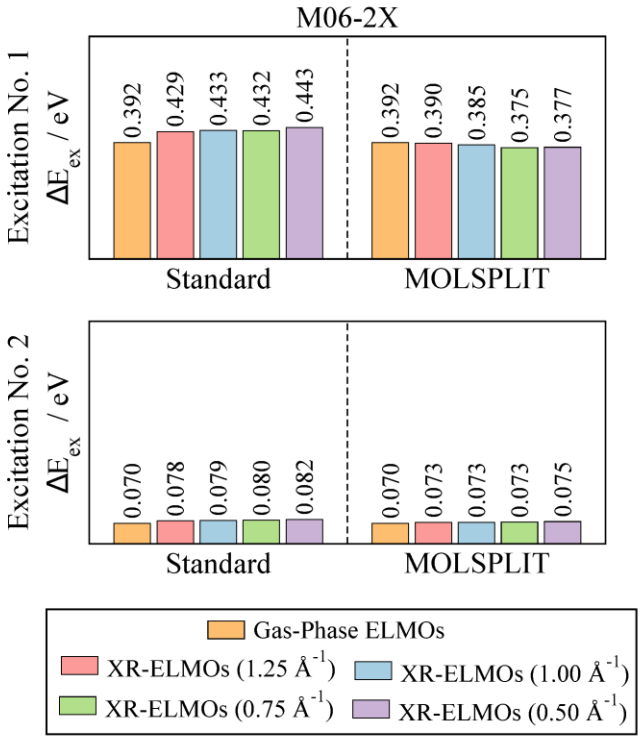

Figure S2 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from EOM-CCSD/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of X-ray datasets associated with periodic M06-2X densities (standard and MOLSPLIT) and characterized by different maximal resolutions (1.25 Å^{-1}, 1.00 Å^{-1}, 0.75 Å^{-1} and 0.50 Å^{-1}).

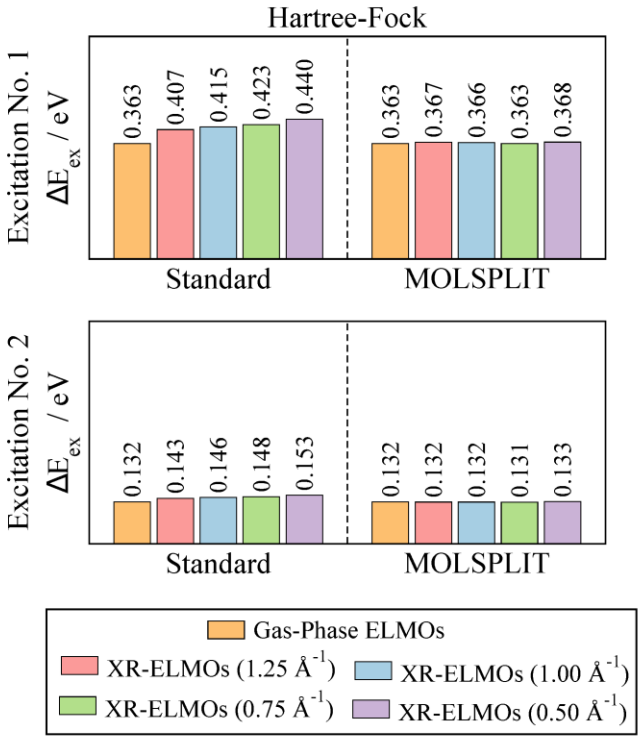

Figure S3 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from TFDDFT/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of X-ray datasets associated with periodic Hartree-Fock densities (standard and MOLSPLIT) and characterized by different maximal resolutions (1.25 $Å^{-1}$, 1.00 $Å^{-1}$, 0.75 $Å^{-1}$ and 0.50 $Å^{-1}$).

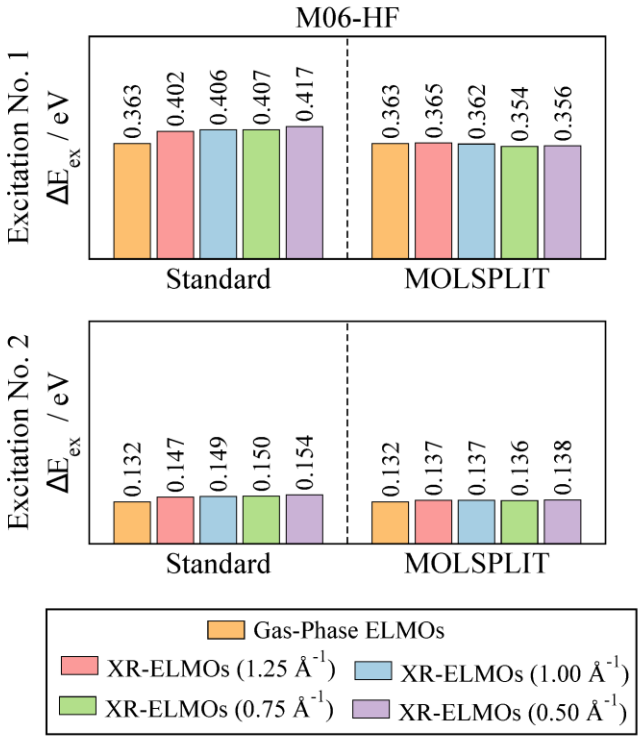

Figure S4 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from TDDFT/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of X-ray datasets associated with periodic M06-HF densities (standard and MOLSPLIT) and characterized by different maximal resolutions (1.25 Å^{-1}, 1.00 Å^{-1}, 0.75 Å^{-1} and 0.50 Å^{-1}).

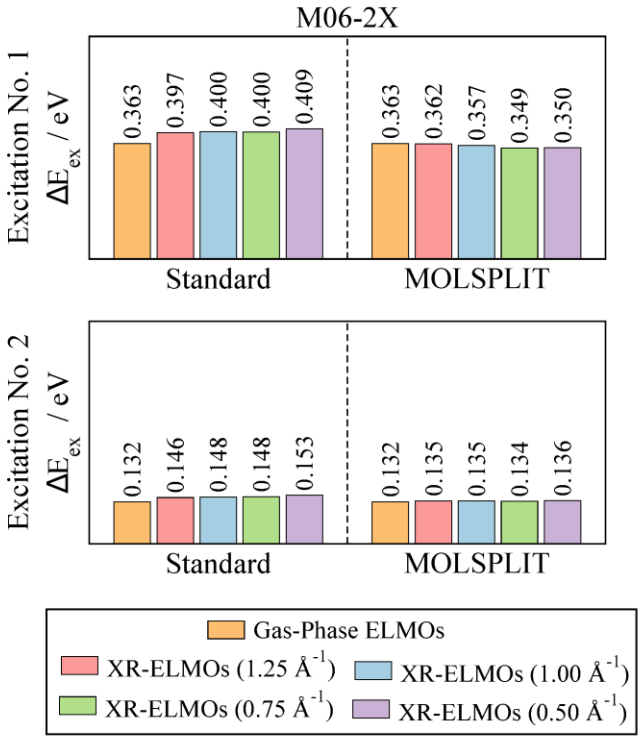

Figure S5 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from TDDFT/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of X-ray datasets associated with periodic M06-2X densities (standard and MOLSPLIT) and characterized by different maximal resolutions (1.25 $Å^{-1}$, 1.00 $Å^{-1}$, 0.75 $Å^{-1}$ and 0.50 $Å^{-1}$).

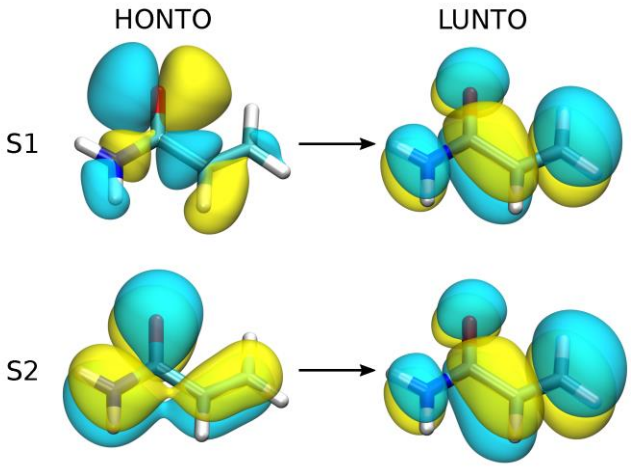

Figure S6 HONTOs (highest occupied natural transition orbitals) and LUNTOs (lowest unoccupied natural transition orbitals) associated with the first and the second excited states of acrylamide (here labelled as S1 and S2, respectively), as resulting from the gas-phase calculation at TDDFT (CAM-B3LYP) level with basis-set cc-pVDZ; all the isosurfaces set to 0.02 a.u.

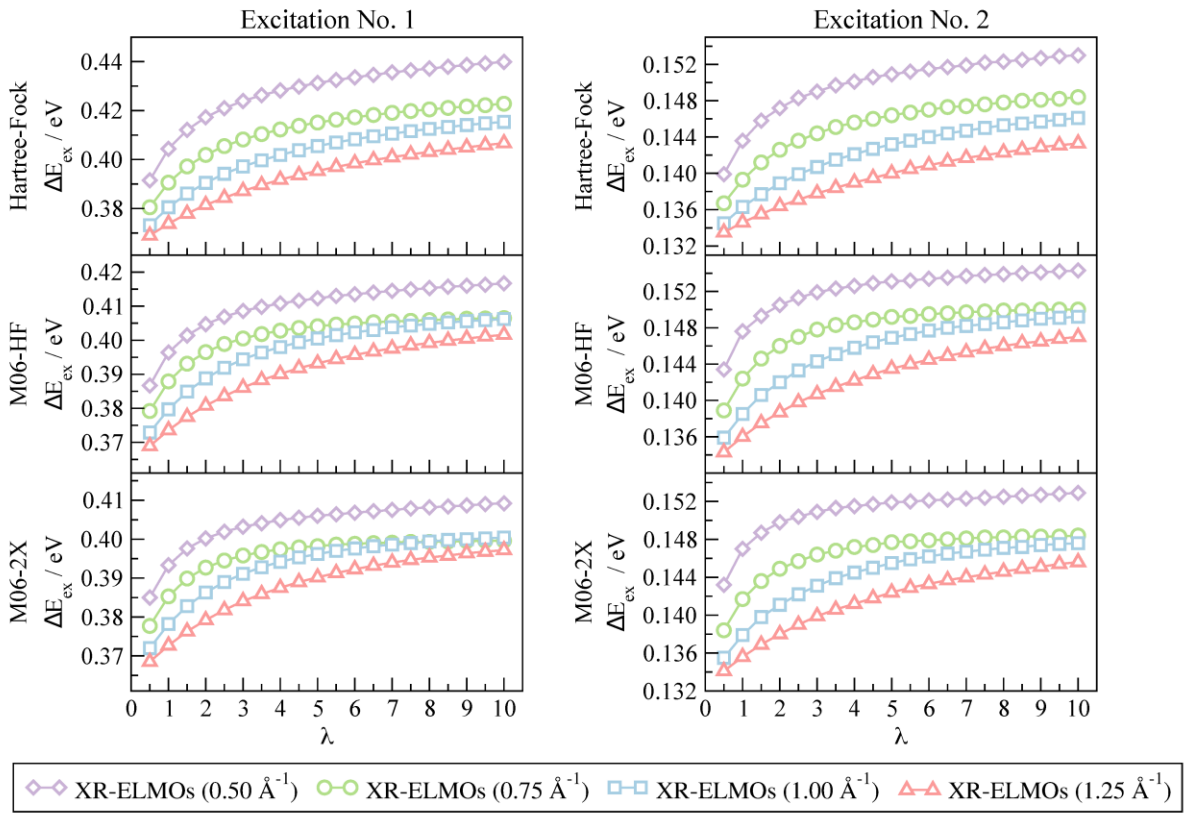

Figure S7 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as obtained through TDDFT/ELMO calculations with embedding XR-ELMOs. The variations are reported as a function of the λ value used in the preliminary calculations of the embedding XR-ELMOs at different resolutions (1.25 $Å^{-1}$, 1.00 $Å^{-1}$, 0.75 $Å^{-1}$ and 0.50 $Å^{-1}$) and levels of theory (standard Hartree-Fock, M06-HF and M06-2X).

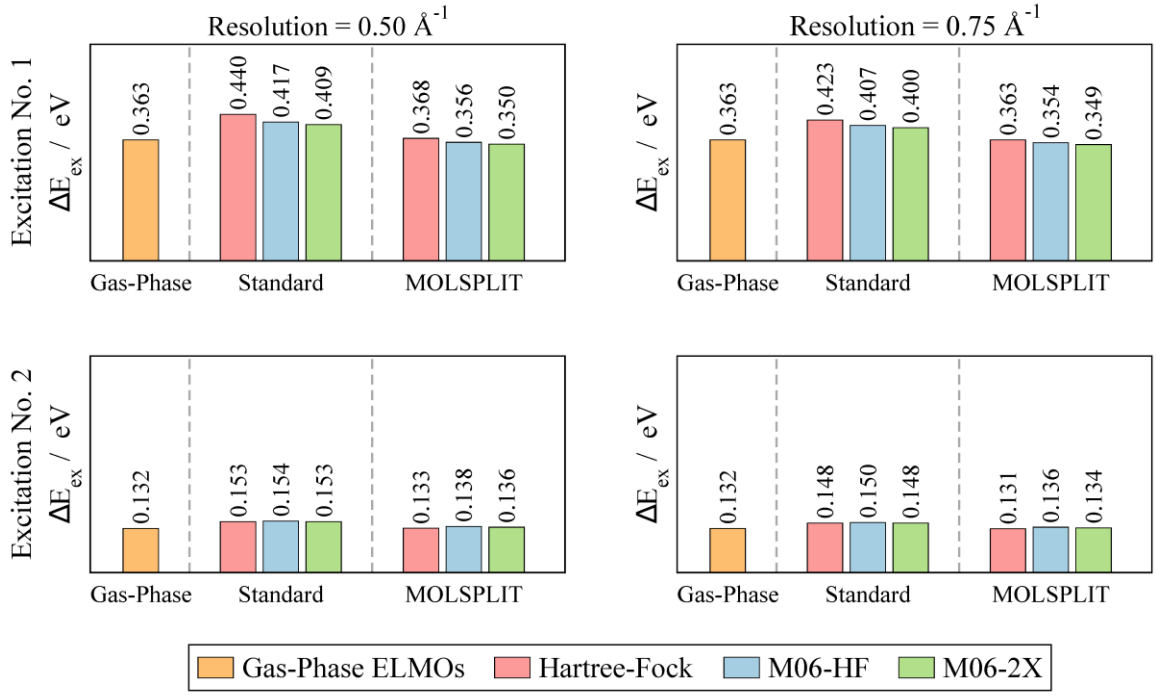

Figure S8 Variations of the excitation energies (ΔE_{ex}) for the first two excited states of acrylamide with respect to the corresponding gas-phase values, as resulting from TDDFT/ELMO calculations with embedding gas-phase ELMOs and with embedding XR-ELMOs obtained through XRW fittings ($\lambda = 10.0$) of structure factor amplitudes computed at different levels of theory (Hartree-Fock, M06-HF, M06-2X, MOLSPLIT-Hartree-Fock, MOLSPLIT-M06-HF and MOLSPLIT-M06-2X). The results are shown for two resolutions of the X-ray datasets (0.50 Å^{-1} and 0.75 Å^{-1}).