Supporting Information for :

C K-edge NEXAFS spectra of graphene with physical and chemical defects: A study based on density functional theory

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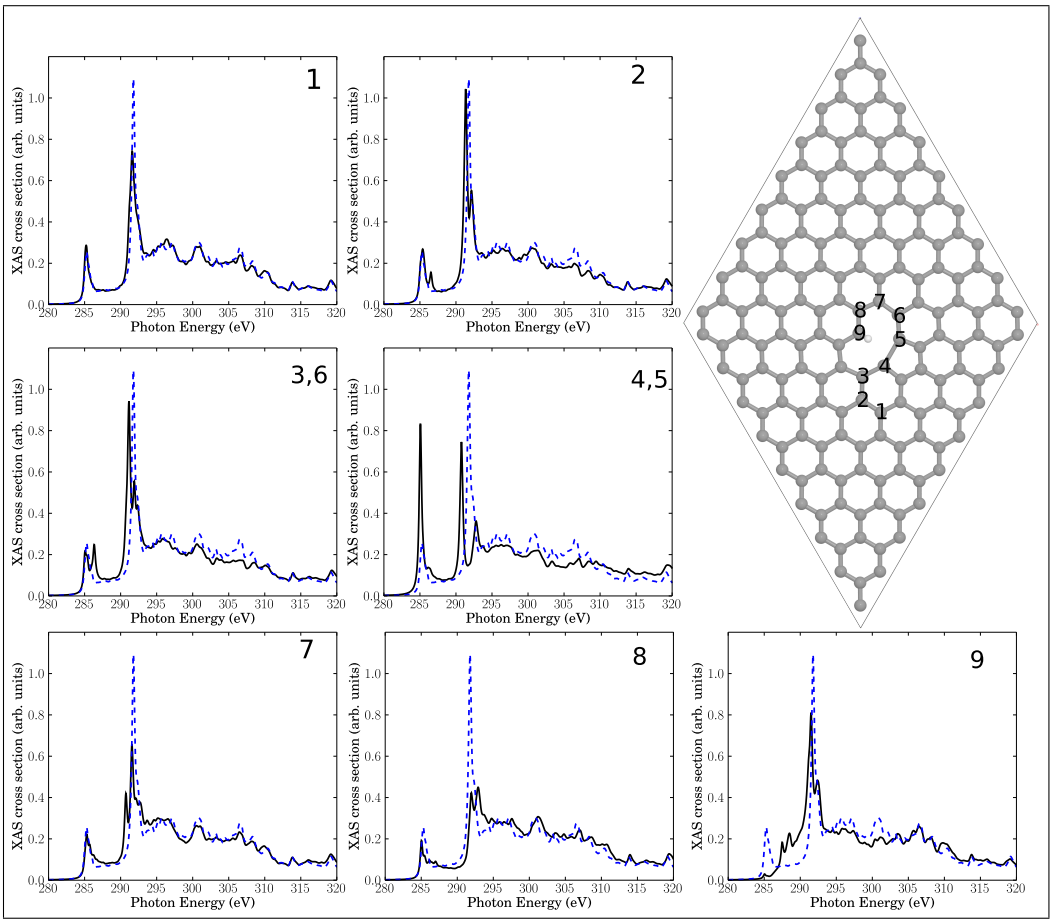
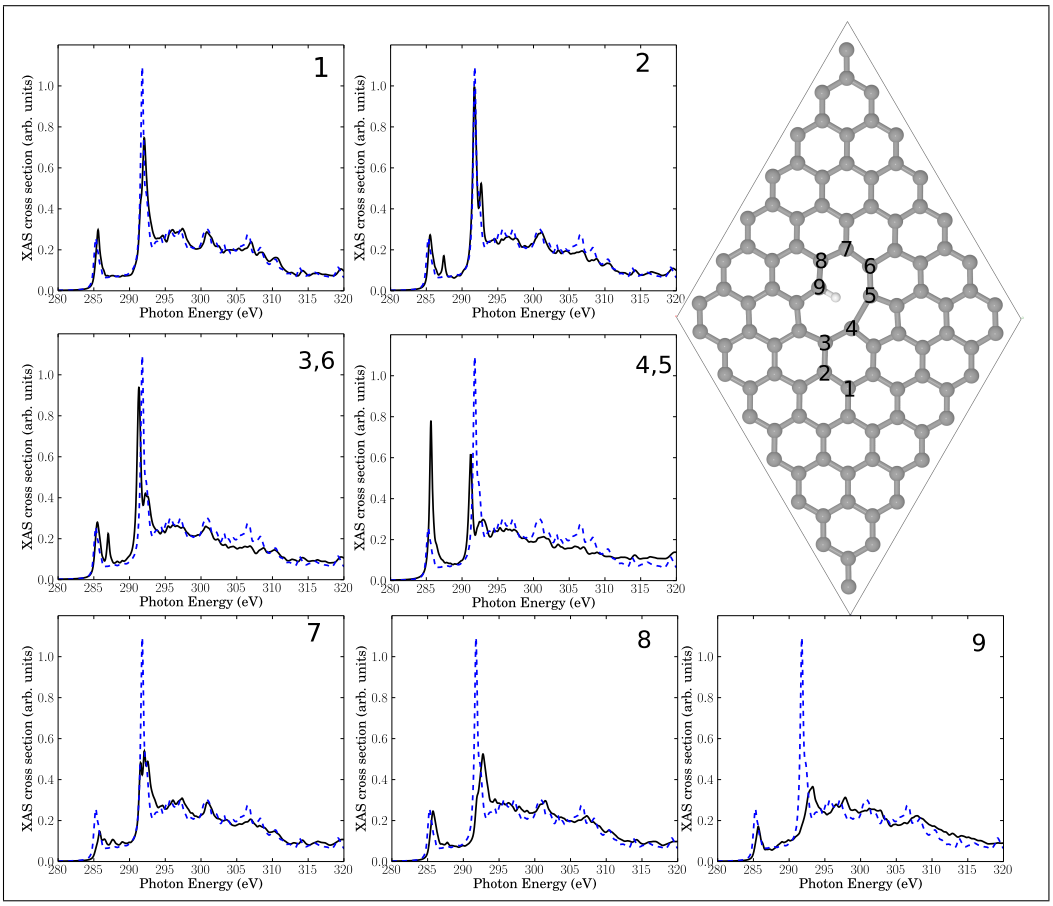
The following two figures demonstrate the results of additional test calculations, for the single-vacancy case, as reported towards the end of section 3.2.2 in the main text. The first figure Fig_SI 1 shows NEXAFS spectra for a larger unit cell, 9×9, to be compared to the results obtained with 7×7 in Fig.4 of the main text. The second figure Fig_SI 2 shows NEXAFS spectra for the case when this defect was decorated with a single rather than two, H atoms.



Fig_SI 1: Upper right: Single-vacancy (V_1(5,9)) defect, decorated with two H atoms (both at C atom 9), in a 9×9 cell. The seven insets show NEXAFS spectra corresponding to core-hole creation in atoms 1-9, located close to the defect. Full, black lines: Computed NEXAFS spectra, dashed, blue lines: The theoretical spectrum of unperturbed graphene for comparison.



Fig_SI 2: Upper right: Single-vacancy (V_1(5,9)) defect, decorated with one H atom (at C atom 9), in a 7×7 cell. The seven insets show NEXAFS spectra corresponding to core-hole creation in atoms 1-9, located close to the defect. Full, black lines: Computed NEXAFS spectra, dashed, blue lines: The theoretical spectrum of unperturbed graphene for comparison.