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Supporting Information

Accurate K-edge X-ray photoelectron and absorption spectra of g-C_3N_4 nanosheet by first-principles simulations and reinterpretations

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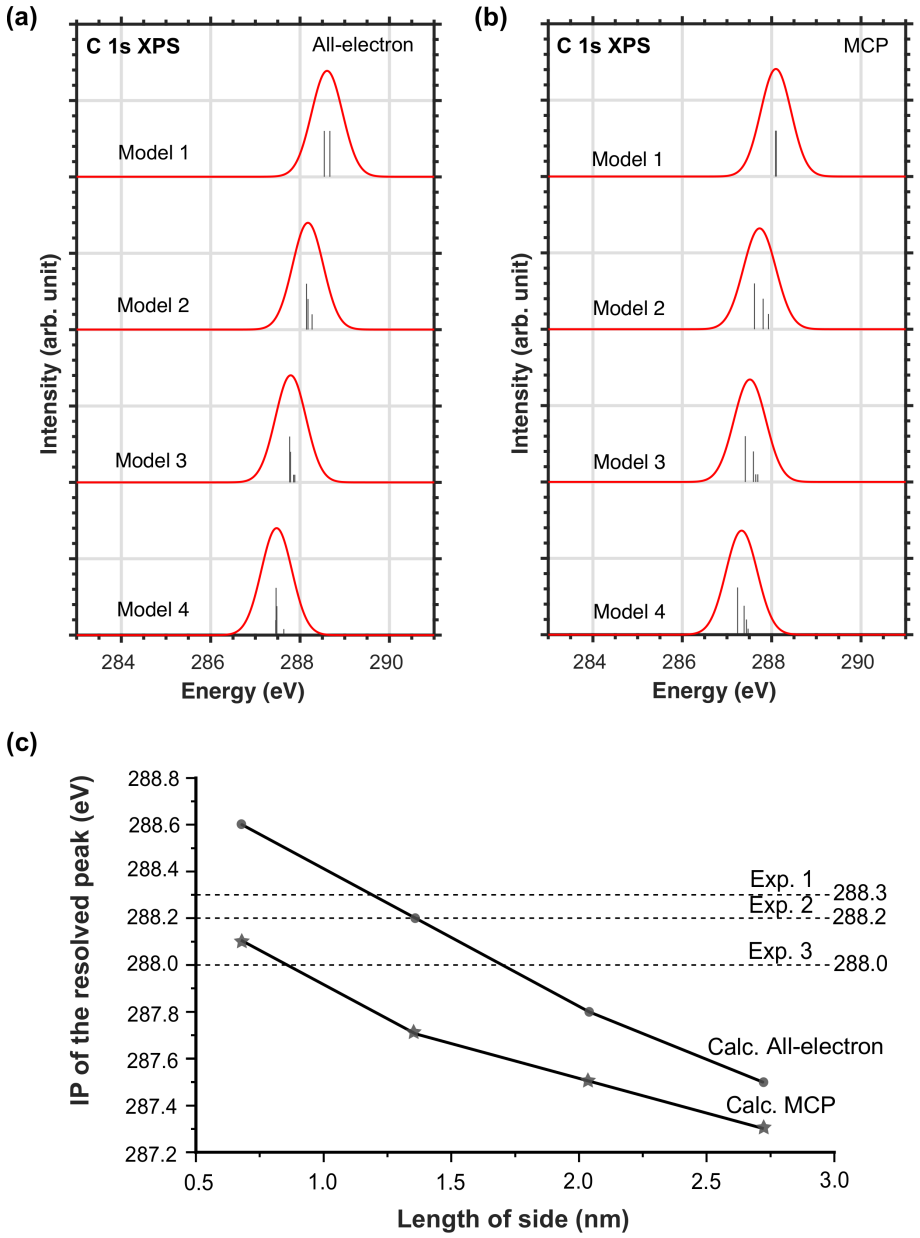

Figure S1 Simulated C1s XPS spectra for four models of g-C_3N_4 nanosheets, where each nitrogen was represented by (a) an all-electron atom (recaptured from Fig. 4b in the main text) and (b) model core potential (MCP) with 1s electrons removed. Each vertical stick denotes N1s IP with length scaled according to its atomic weight. (c) Resolved main peak position at different model size: Comparison of the two methods. The two methods lead to similar (differing by $\sim$0.2 eV) convergent results, except that the latter gives slightly red-shifted IP and quicker size convergence.

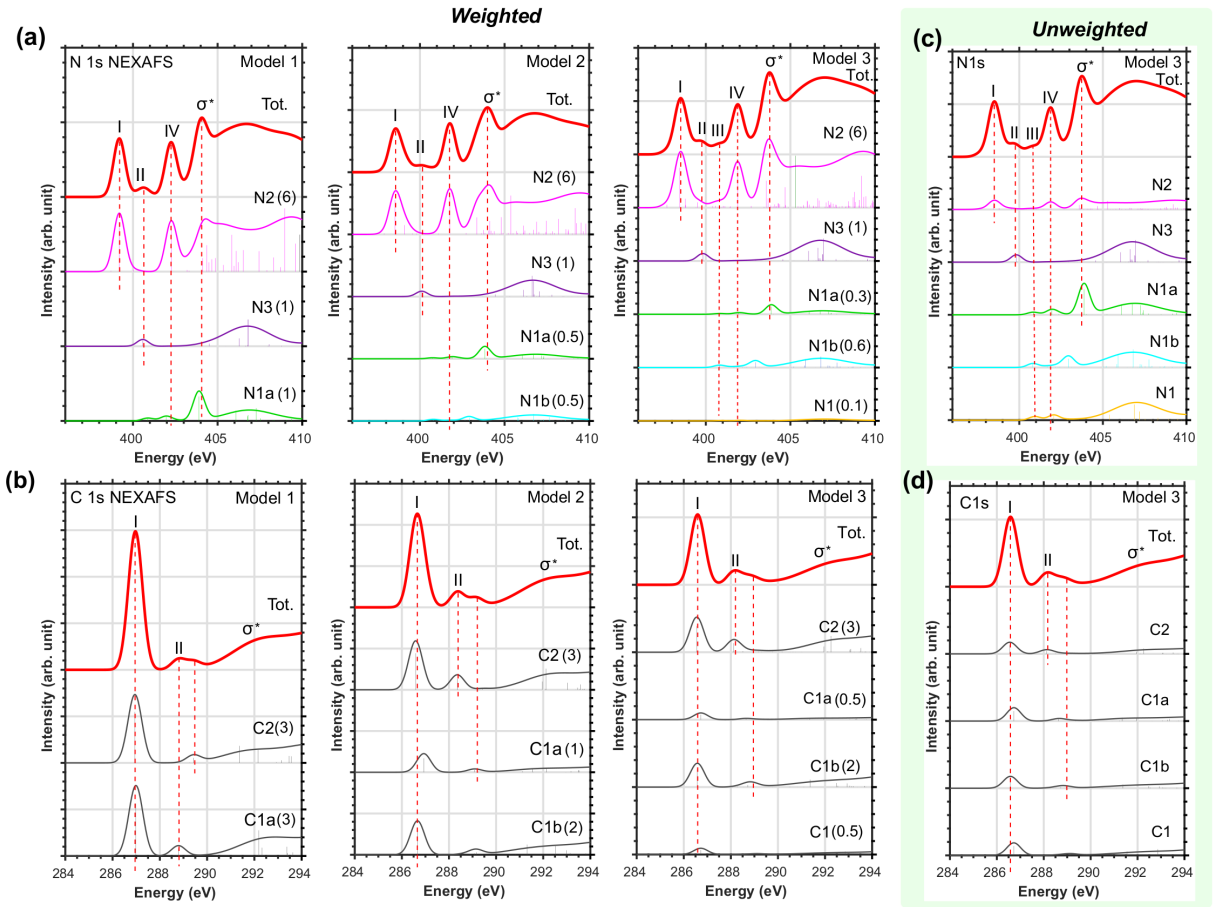

Figure S2 (a-b) Atom-specific contribution analysis for simulated NEXAFS spectra of models 1–3 (left to right): (a) N1s and (b) C1s edge. The spectra were simulated by the B3LYP-ECH method. Each atomic specific spectrum has been scaled with their atomic weight (included in parentheses of the curve label). (c–d) Unweighted results for model 3, for better view of spectra with small weights: (c) N1s and (d) C1s edge. Major peaks are labeled. Dashed lines are to guide eyes.