Electronic Supporting Information for

Carbon Nitride Photocatalysts for Watersplitting; a Computational Perspective

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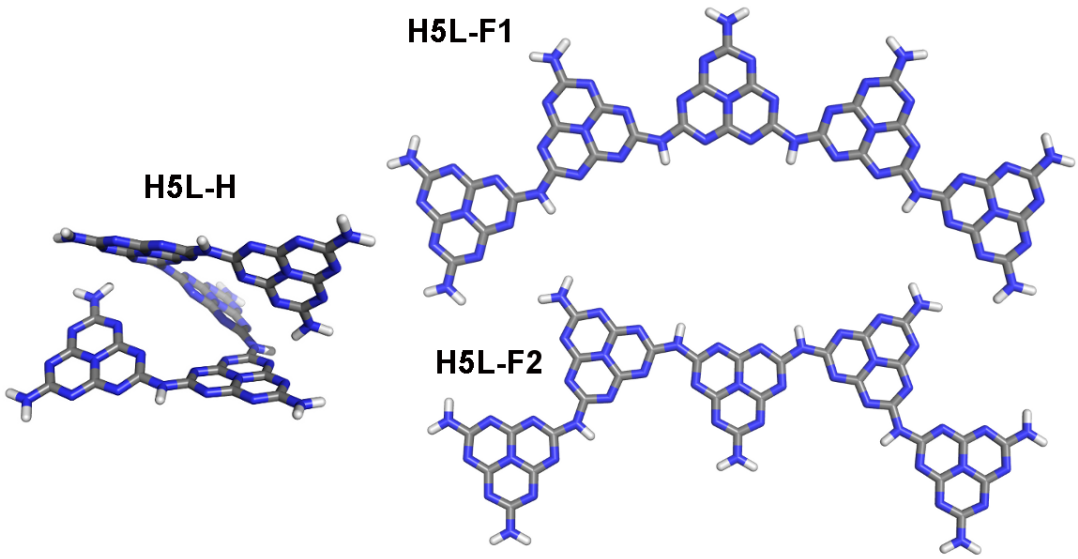

Fig. S1 DFT optimised geometries of the helical and flat conformers of H5L.

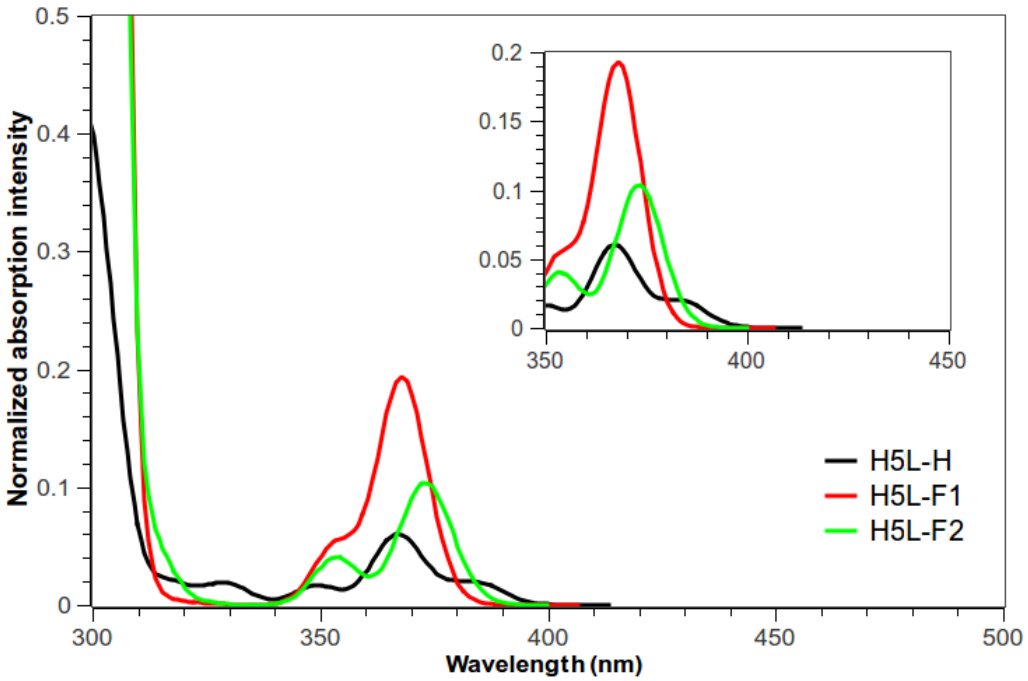

Fig. S2 Comparison of TD-B3LYP predicted spectra of helical and flat conformers of the H5L cluster model.

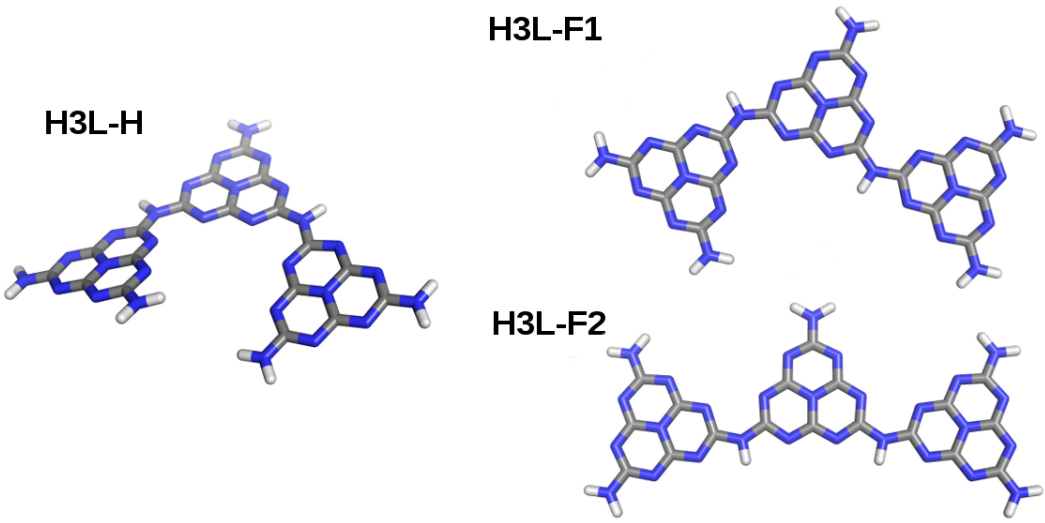

Fig. S3 DFT optimised geometries of the helical and flat conformers of H3L (H3L-F1 is H3L-F in the main paper).

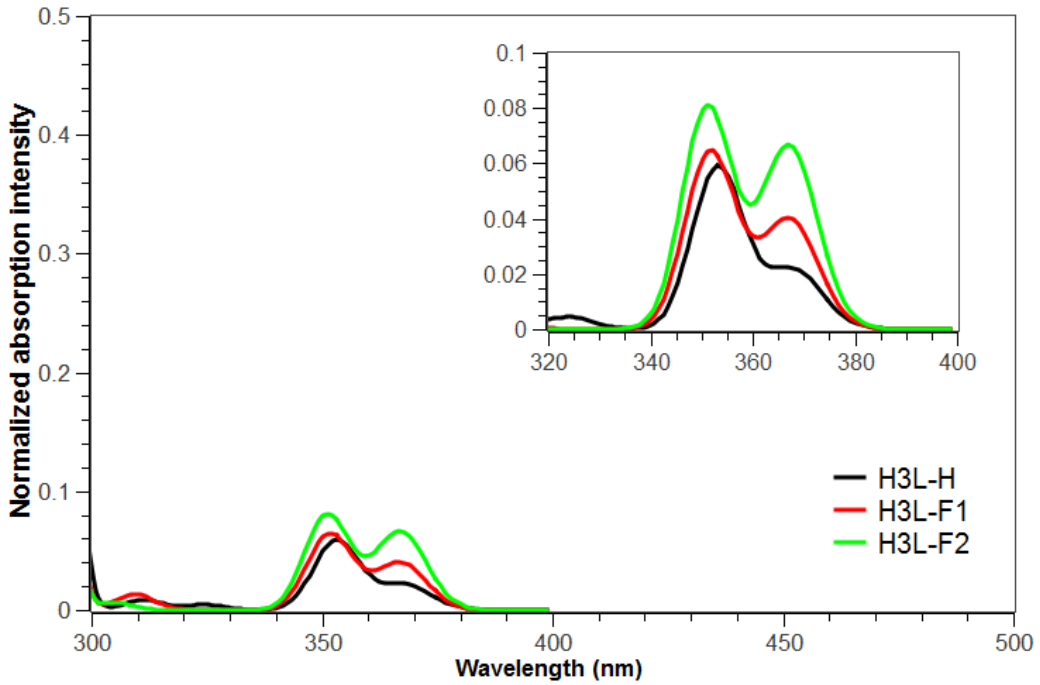

Fig. S4 Comparison of TD-B3LYP predicted spectra of helical and flat conformers of the H3L cluster model.

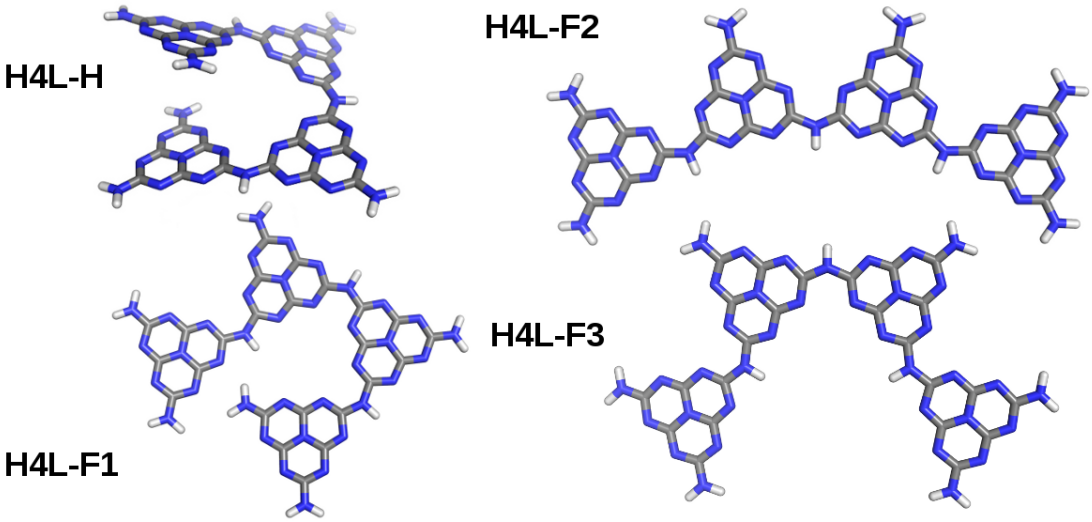

Fig. S5 DFT optimised geometries of the helical and flat conformers of H4L (H4L-F1 is H4L-F in the main paper).

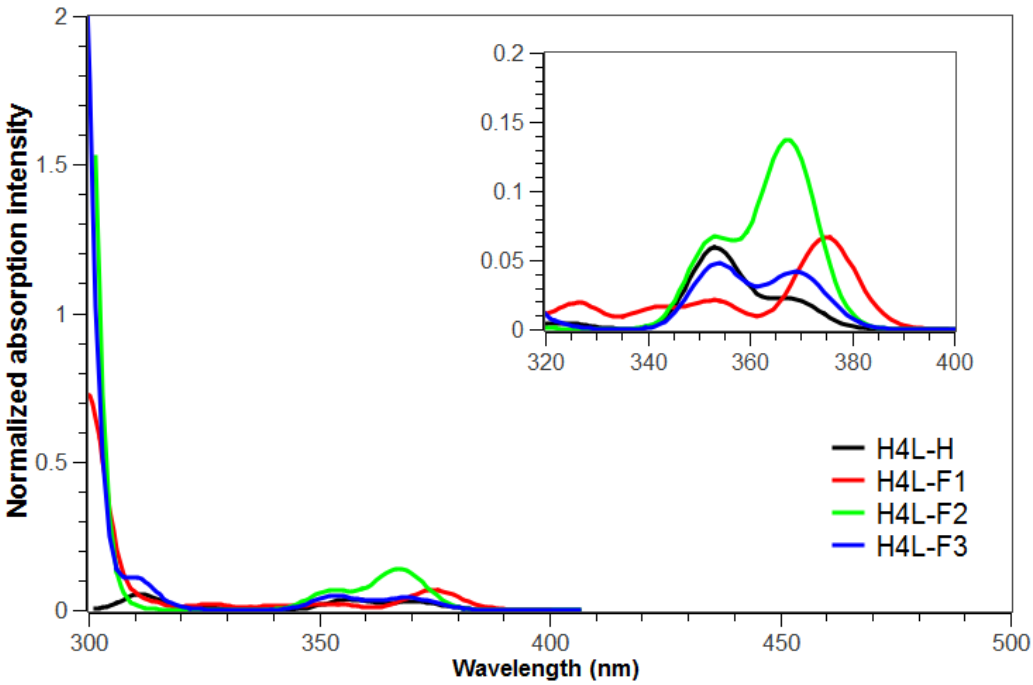

Fig. S6 Comparison of TD-B3LYP predicted spectra of helical and flat conformers of the H4L cluster model.

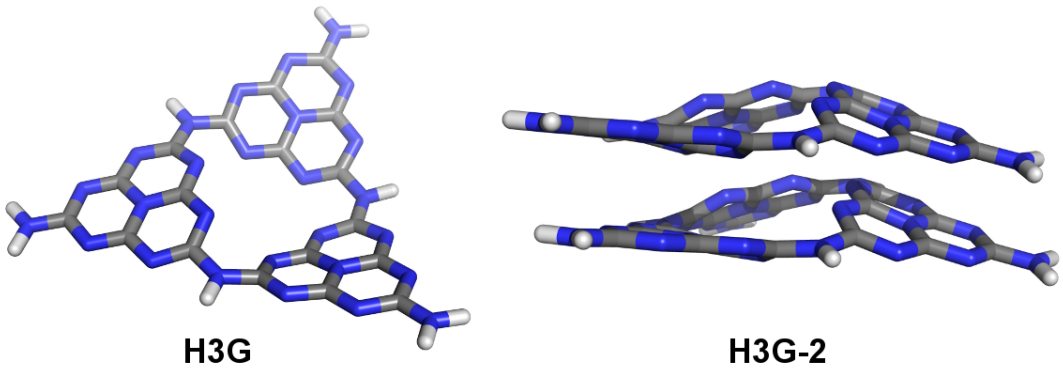

Fig. S7 Comparison of the DFT optimised geometries of an isolated H3G cluster model and a stack of two.

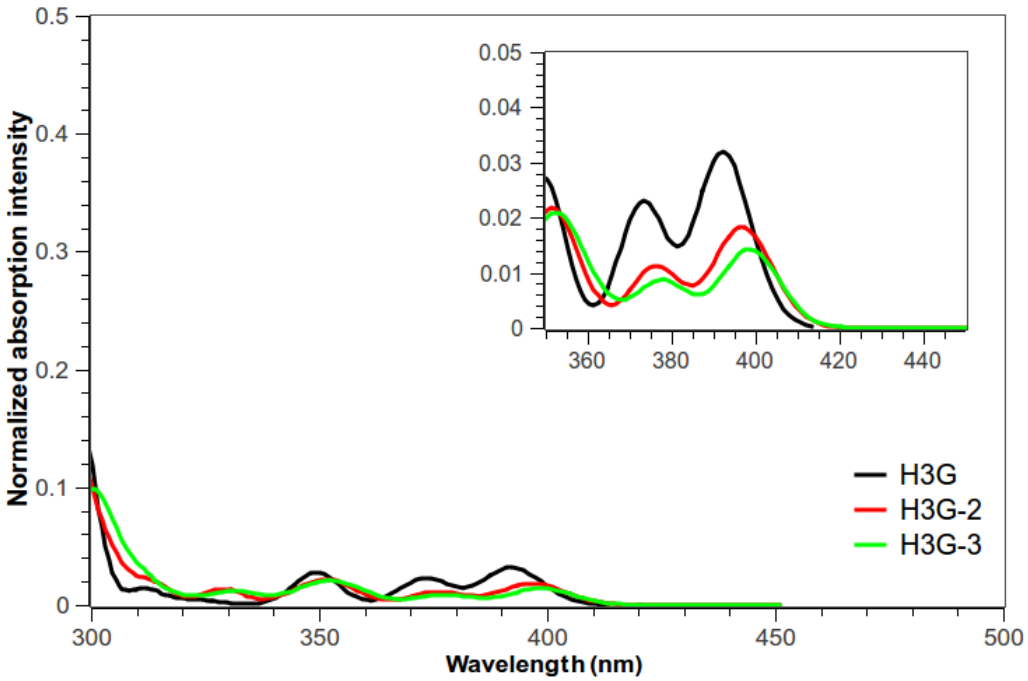

Fig. S8 Effect of the effect of stacking on the TD-B3LYP predicted spectra of H3G.

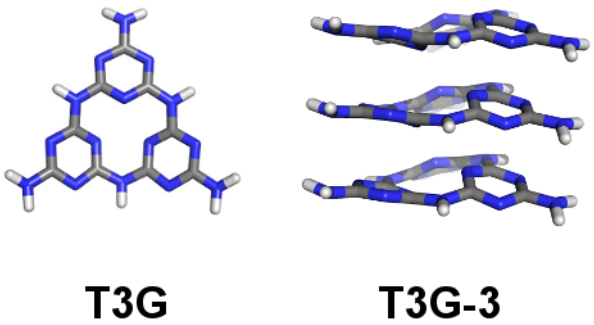

Fig. S9 Comparison of the DFT optimised geometries of an isolated T3G cluster model and a stack of three.

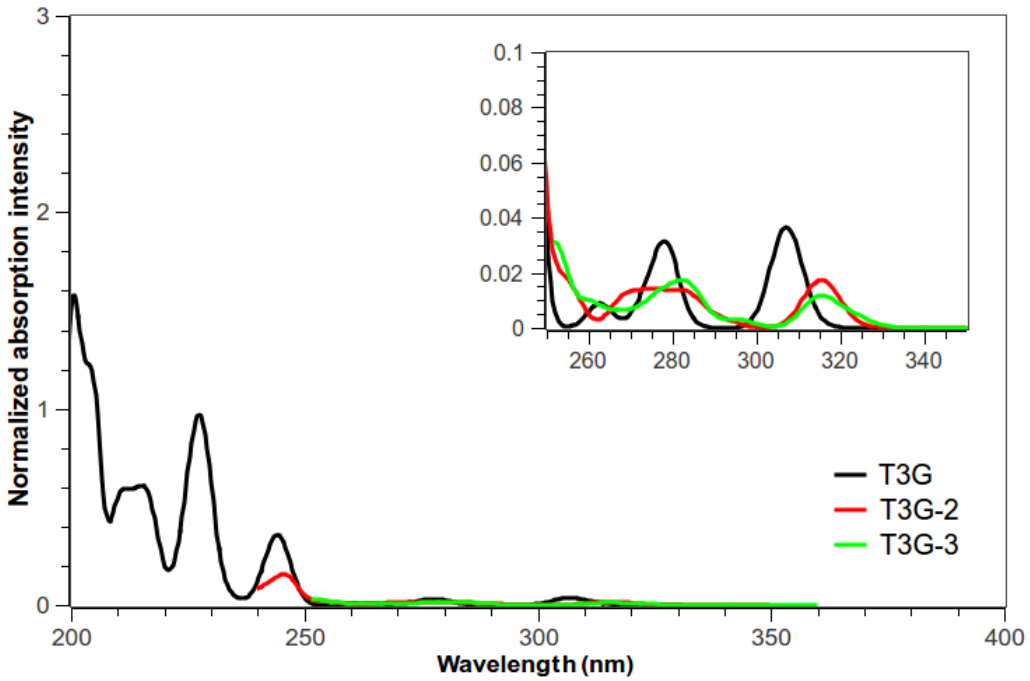

Fig. S10 Effect of the effect of stacking on the TD-B3LYP predicted spectra of T3G.

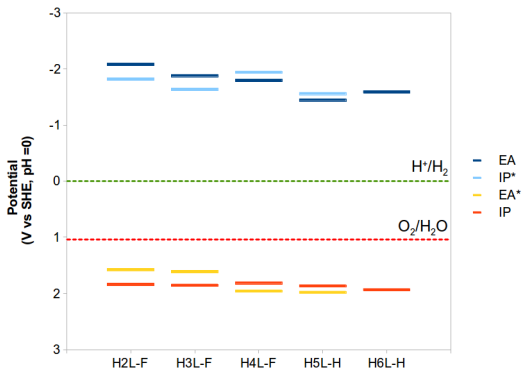

Fig. S11 (TD-)B3LYP predicted IP, EA, IP* and EA* adiabatic potentials of the lowest energy conformers of cluster models of linear heptazine-based structures in water (ε = 80.1) at pH 0.

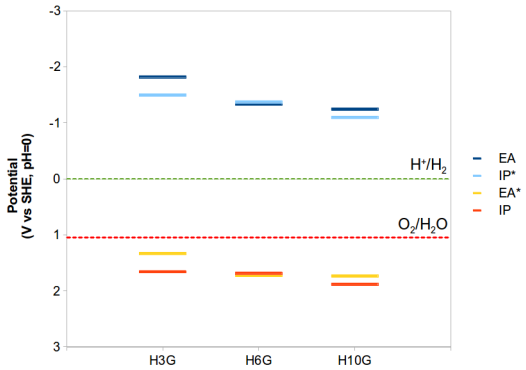

Fig. S12 (TD-)B3LYP predicted IP, EA, IP* and EA* adiabatic potentials of the lowest energy conformers of cluster models of graphitic heptazine-based structures in water (ε = 80.1) at pH 0.

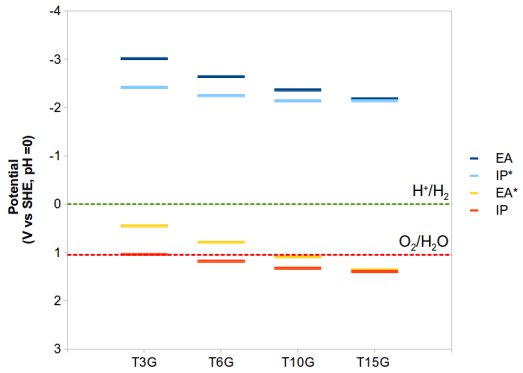

Fig. S13 (TD-)B3LYP predicted IP, EA, IP* and EA* adiabatic potentials of the lowest energy conformers of cluster models of graphitic triazine-based structures in water (ε = 80.1) at pH 0.

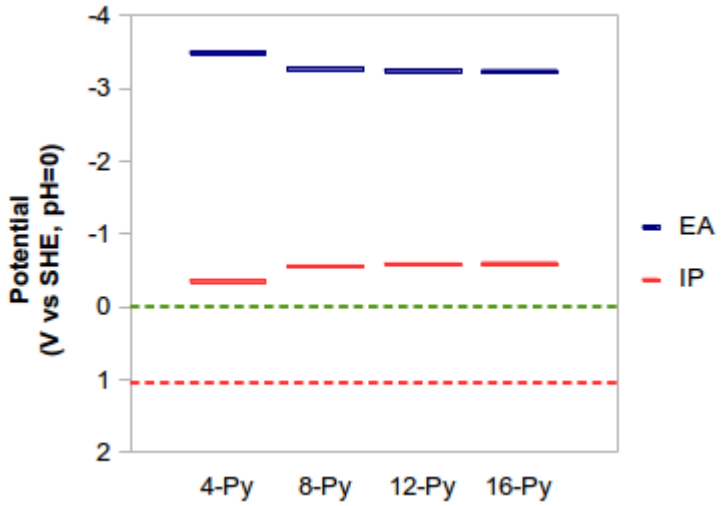

Fig. S14 Comparison of the alignment of the EA and IP potentials of polypyrrole chains of 4 to 16 pyrrole units in water (ε = 80.1) at pH 7.

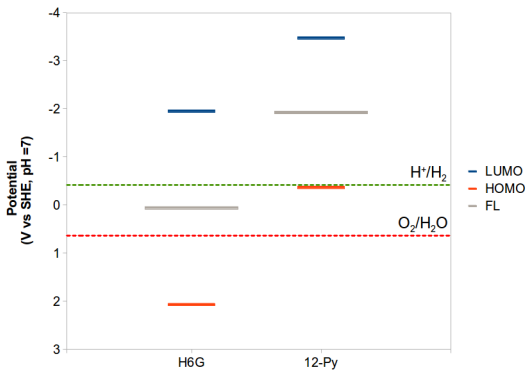

Fig. S15 Alignment of the top of the valence band (HOMO) and bottom of conduction band (LUMO) of carbon nitride (H6G) and polypyrrole (12-Py) in water (ε = 80.1) at pH 7 (Kohn-Sham orbital equivalent of Fig. 16 in the main paper).