## Designing Half-metallic Ferromagnetism by A New Strategy: The Example of Superhalogens Modified Graphitic C<sub>3</sub>N<sub>4</sub>

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 $\begin{array}{c} \mbox{Figure S1 Spin-resolved band structures and 3D isosurface plots of spin charge density for g-} \\ C_3N_4 & \mbox{doped} & \mbox{by} & \mbox{holes.} \end{array}$ 



Figure S2 Spin-resolved (a) band structures and (b) partial density of states of  $g-C_3N_4BF_4$ . (c) Top and side view of 3D isosurface plots of spin charge density for  $g-C_3N_4BF_4$ .



Figure S3 Variation of the total magnetic moment per  $(C_3N_4)_4BF_4$  and  $C_3N_4BF_4$  formula unit as a function of temperature obtained from Monte Carlo simulations based on the Ising model.



Figure S4 Fluctuations of ferromagnetic moment as a function of molecular dynamic simulation steps at 300 K.