

Supporting information for

DFT calculations for single-atom confinement effects of noble metals on monolayer g-C₃N₄ for photocatalytic applications

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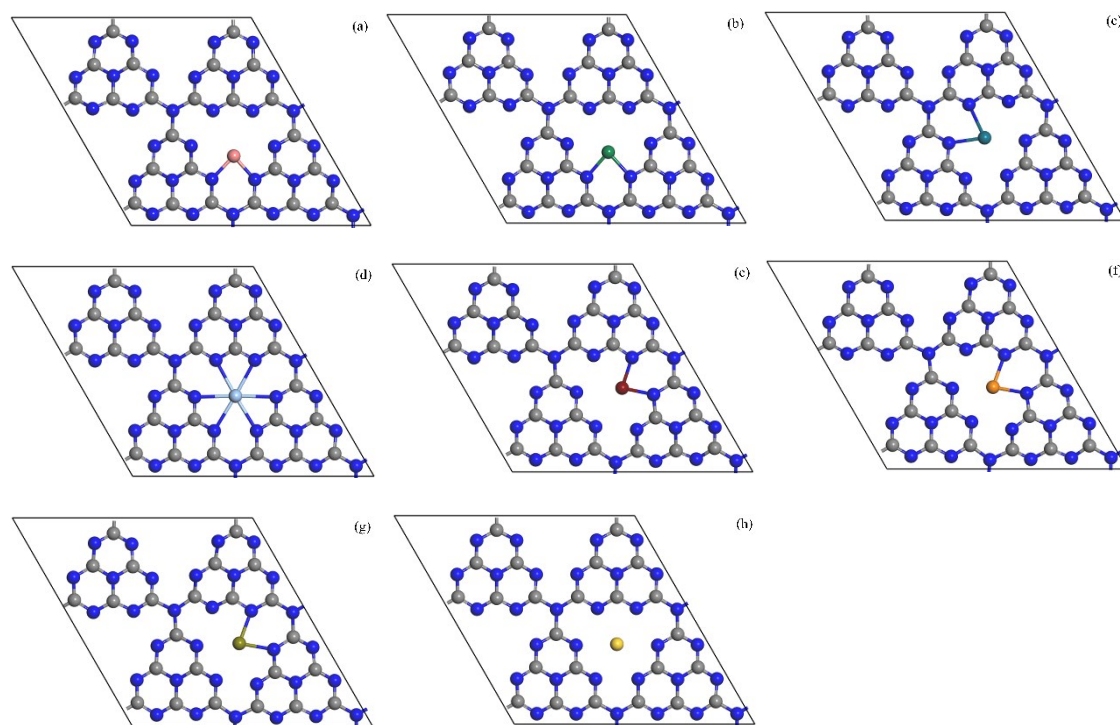


Fig.S1 Top view of optimized structure for NM1@g-C₃N₄, NM=(a) Ru, (b) Rh, (c) Pd, (d) Ag, (e) Os, (f) Ir, (g) Pt, (h) Au. The balls in gray and blue represent the C and N atoms, respectively.

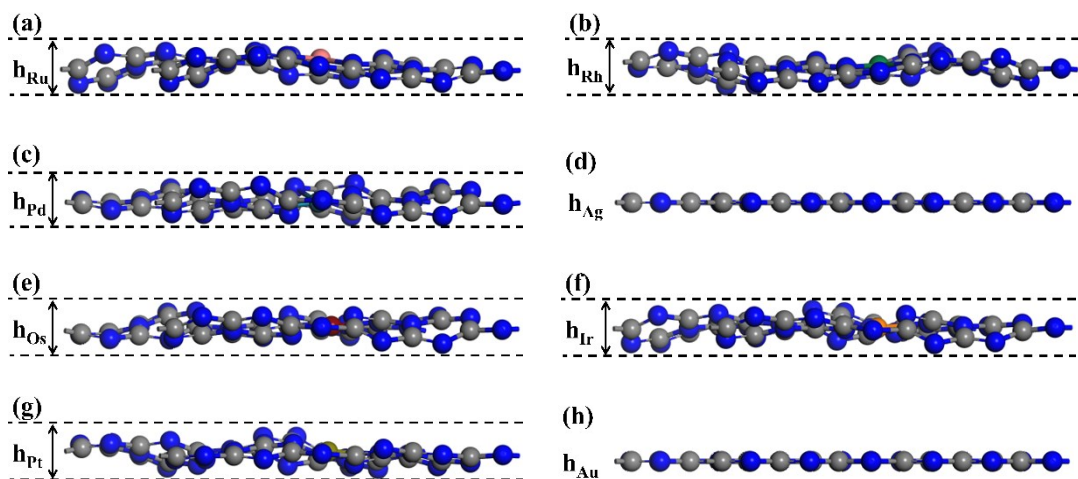


Fig.S2 Side view of optimized structure for NM1@g-C3N4, NM=(a) Ru, (b) Rh, (c) Pd, (d) Ag, (e) Os, (f) Ir, (g) Pt, (h) Au. The balls in gray and blue represent the C and N atoms, respectively.