

## “Supplementary Materials”

### **Catalytic role of graphitic nitrogen atoms in CO oxidation reaction over N-containing graphene: a first-principles mechanistic evaluation**

**Mehdi D. Esrafil<sup>\*,a</sup>, Parisasadat Mousavian<sup>a,b</sup>**

<sup>a</sup> Department of Chemistry, Faculty of Basic Sciences, University of Maragheh, P.O. Box 55136-553, Maragheh, Iran

<sup>b</sup> Department of Chemistry, Azarbaijan Shahid Madani University, Tabriz, Iran

\* Corresponding author. **E-mail:** [esrafil@maragheh.ac.ir](mailto:esrafil@maragheh.ac.ir) (M. D. Esrafil).

**Figure S1.** (a) Coadsorbed configuration of O<sub>2</sub>/CO and the related adsorption energy, and (b) the energy profile and relevant bond distances (in Å) for the formation of OOCO intermediate through the LH mechanism on N<sub>4</sub>-Gr

