

*Supporting Information for*

**Can Metal-Free Silicon-Doped Hexagonal Boron Nitride Nanosheet and  
Nanotube Exhibit Activity toward CO Oxidation?**

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**Figure S-1.** Side and top views for the configurations of initial state (IS), transition state (TS), intermediate state (INT) and final state (FS) with the calculated energies (eV) during CO oxidation following Langmuir–Hinshelwood mechanism on two Si atoms doped h-BNNS.

