A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheet

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Fig. S1 Top and side views of the various O₂ adsorption configurations over V_B/BN. The adsorption energies are also presented in the pictures as insert. The pink, blue and red spheres represent B, N and O, respectively.

(a) \( E_{\text{ads}} = 1.70 \text{ eV} \)

(b) \( E_{\text{ads}} = 0.27 \text{ eV} \)

(c) \( E_{\text{ads}} = 0.20 \text{ eV} \)

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