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Computational Design of Bimetallic (Au-Cu & Ag-Cu) Catalyst for Low Temperature CO Oxidation[1] ALTAF KARIM[2], COMSATS Institute of Information Technology Islamabad Pakistan, ABDUL RAUF, University of Engineering and Technology Lahore Pakistan , AKHTAR HUSSAIN[3], National Center for Physics Islamabad Pakistan — Au–Cu and Ag-Cu bimetallic surfaces are reported to be much more active in CO oxidation than the mono-metallic Pt, Cu, Au, & Ag in our work. First, we used theoretical and experimental results of CO oxidation on Pt surfaces to benchmark and optimize our multiscale modeling framework. Further, we extended this framework to examine the molecular oxygen adsorption, decomposition, and CO oxidation upon a number of Cu modified Au surfaces cleavaged in (100) orientation. The amount of Cu was varied on the Au slab to optimize the model that serves as the best one to investigate the synergic effect between Au and Cu for CO oxidation process. Comparison between different surfaces suggests that the Cu-modified Au surface is superior and more active than pure Cu toward CO oxidation. Similarly, a slab of Ag–Cu having a top monolayer of Cu and three layers beneath is also equally active as Au-Cu. Computational and experimental results show that these surfaces are good candidates for low-temperature CO oxidation.

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