Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Oxygen Reduction Reaction at 68-Atoms Gold Cluster Supported on Carbon Nanotubes: Theoretical and Experimental Analysis

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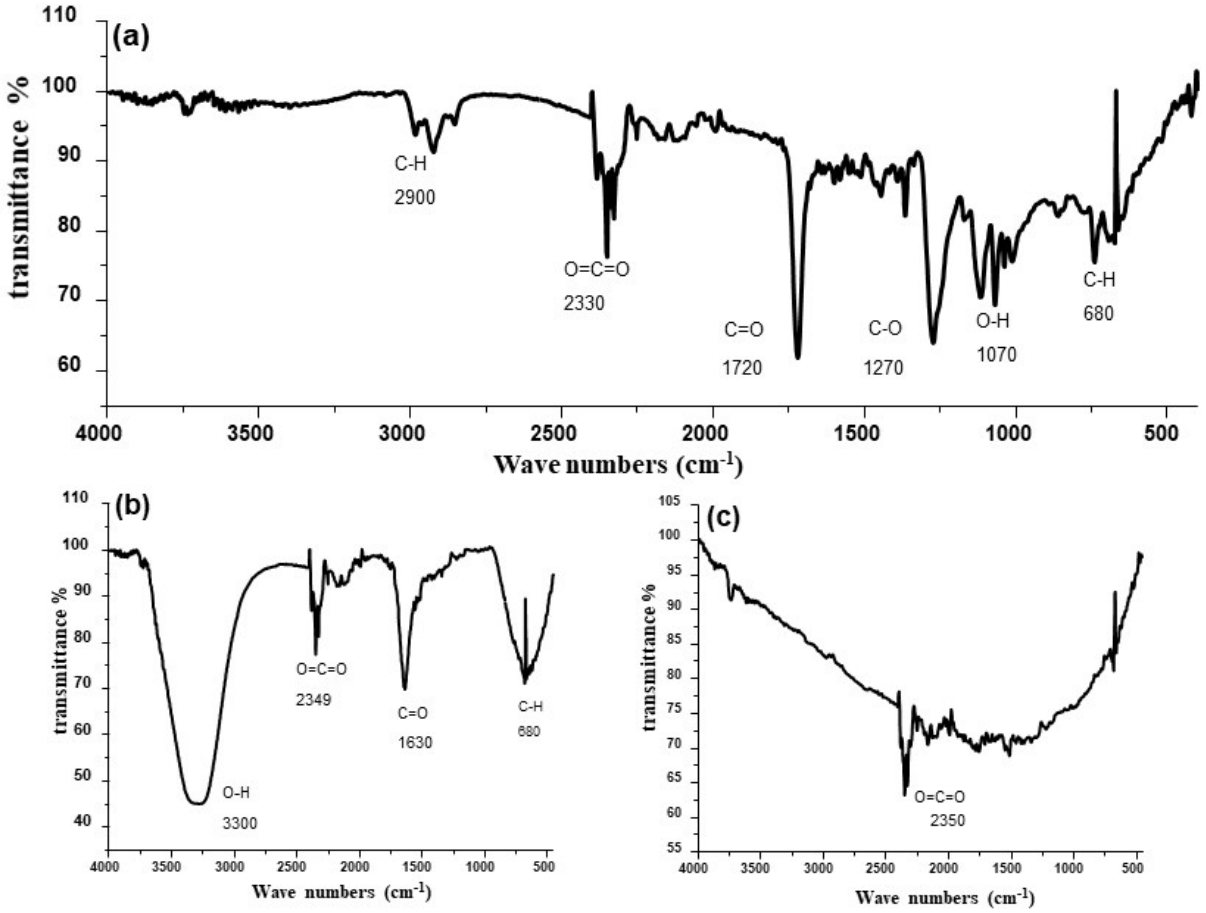

Figure S1. FTIR Spectra for (a) solid Au_{68} nanoparticles with CNT, (b) Au_{68} nanoparticles dispersed in liquid, and (c) carbon nanotubes.

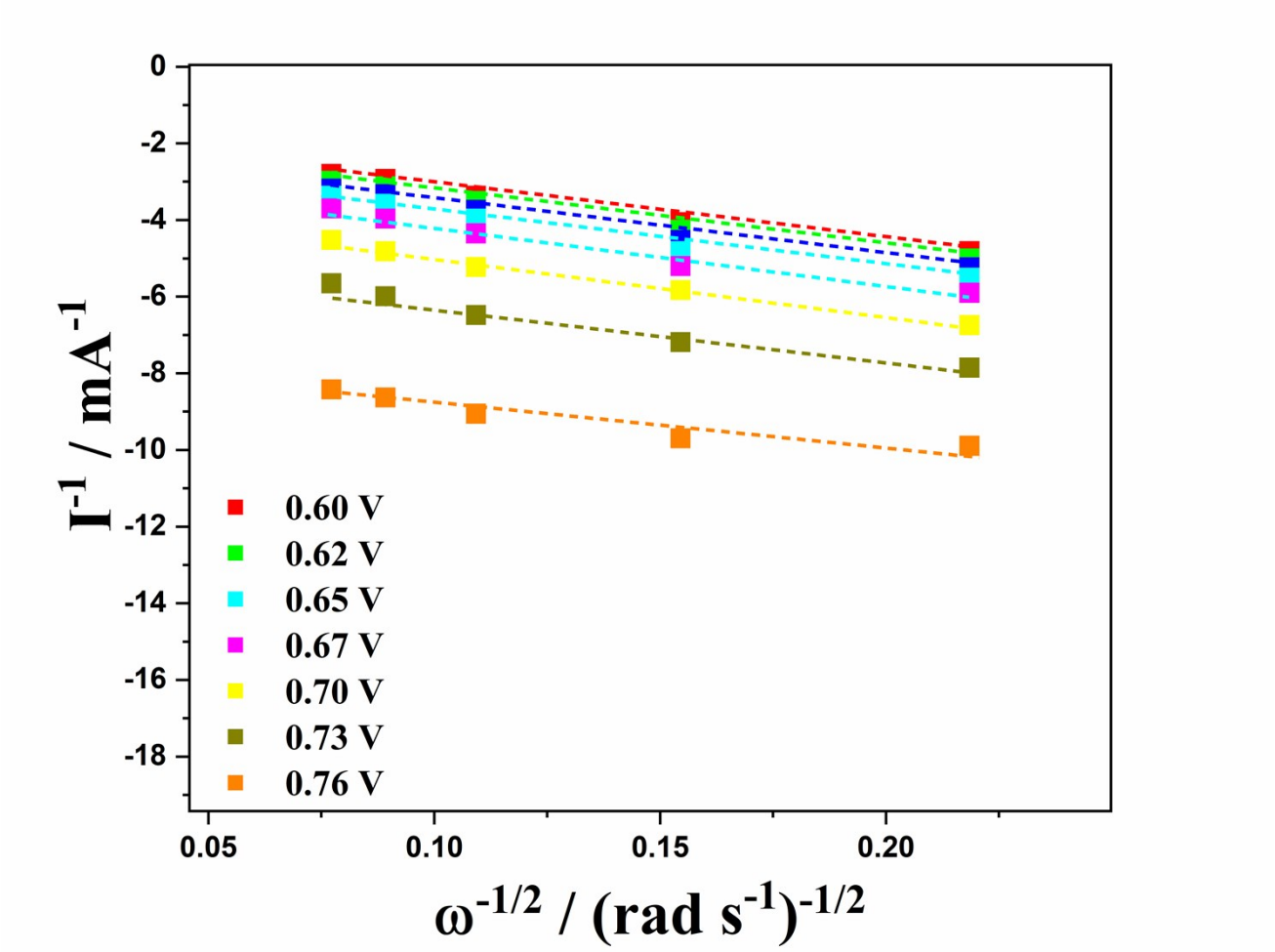

Figure S2. Koutecky-Levich plot for Au68-MWCNT at different electrode potentials.

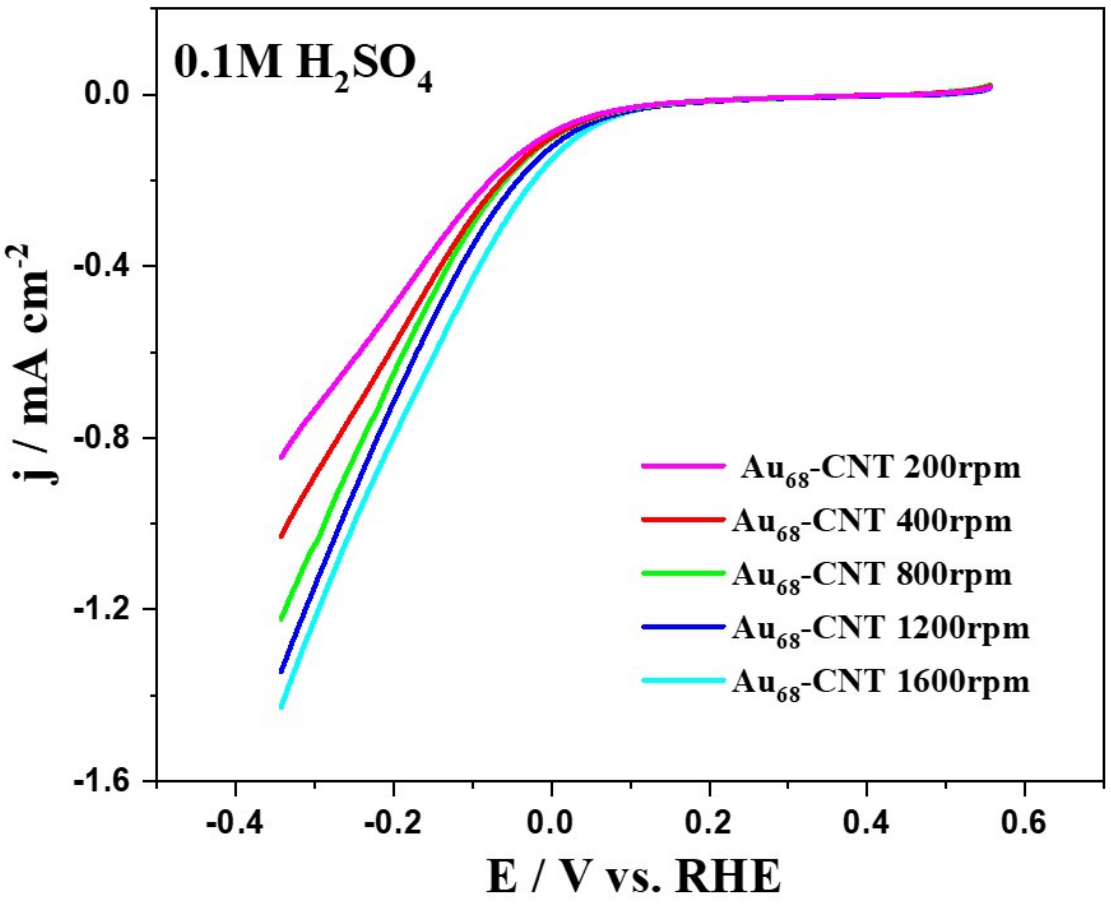

Figure S3. Rotating disk electrode at different r.p.m. in 0.1M H_2SO_4 with O_2-saturated atmosphere and using a scan rate of 5mV s^{-1}.

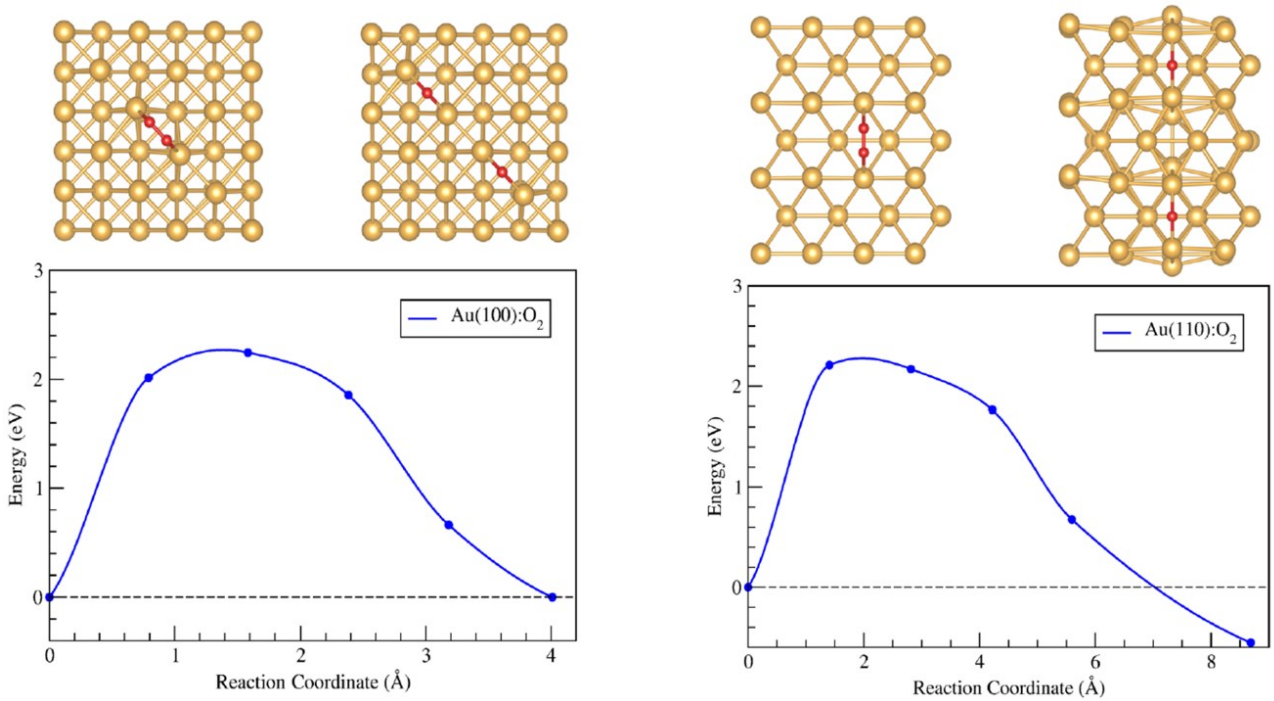

Figure S4. Minimum energy path for the O_2 dissociation on the Au(100) and Au(110) surfaces. The start and end of the reaction coordinate corresponds to the equilibrium positions shown in the figures.

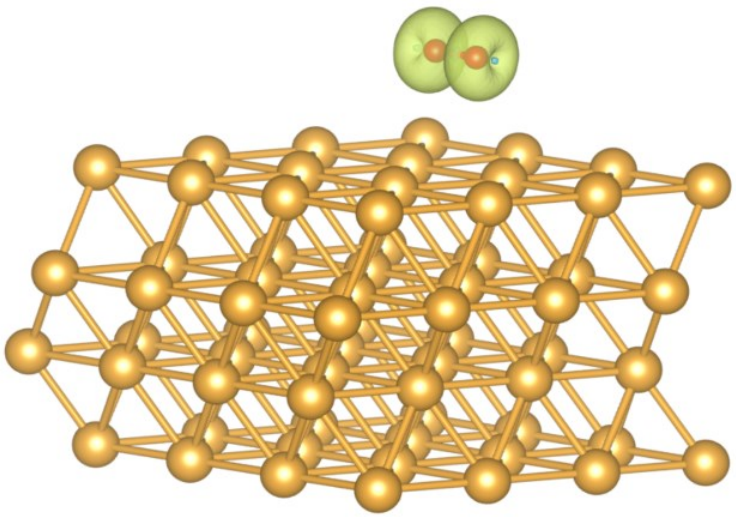

Figure S5. Spin density of O_2 adsorbed on Au(111) surface. Spin-up and spin-down densities are plotted in yellow and blue respectively for an isosurface of $\rho = 1 \times 10^{-3}$ e/Å^3.