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Density Functional Theory Simulation of Cobalt Oxide Aggregation and Facile Synthesis of Cobalt oxide, Gold and Multiwalled Carbon Nanotubes based Ternary Composite for a High Performance Supercapattery

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Raman spectroscopy is the most commonly used non-destructive technique to analyze the quality and structure of the carbon-based materials.[1] **Figure S1 (a and b)** presents the Raman spectra of MWCNTs and Co_3O_4/Au@MWCNTs composite, respectively. In **Figure**

S1(a and b), two sharp peaks at 1356 (1350 cm^{-1} in case of composite) and 1592 (1585 cm^{-1} in case of composite) cm^{-1} presents the typical defect bands (D) and attributed to the presence of disorder in carbon systems (disorder induced by defects and curvature in the nanotube lattice)[2] and G (graphite)-band owing to the in-plane vibration of the C–C bond (G band), respectively.[3-5] Also, an overtone of the D band (2D band) is present at 2695 cm^{-1} (2708 cm^{-1} in case of composite), attributed to the two-phonon scattering.[6] However, the spectra in **Figure S1b** (and inset) shows significant differences as compared to the pristine MWCNTs and featured several peaks in the lower wavenumber region, mainly ascribed to the presence of Co_2O_3 NPs in the Co_3O_4/Au@MWCNTs ternary composite. It should be noted that Raman does not detect the noble metals and therefore, Au traces cannot be seen in the spectra.[7] The peaks present at 479, 520,622 and 686 cm^{-1} are attributed to E_g, F^1_{2g}, F^2_{2g} and A_{1g} modes of modes of Co_3O_4, respectively.[7-9] Hence, the Raman spectra compliments the other results in the manuscript and shows the successful formation of Co_3O_4/Au@MWCNTs composite.

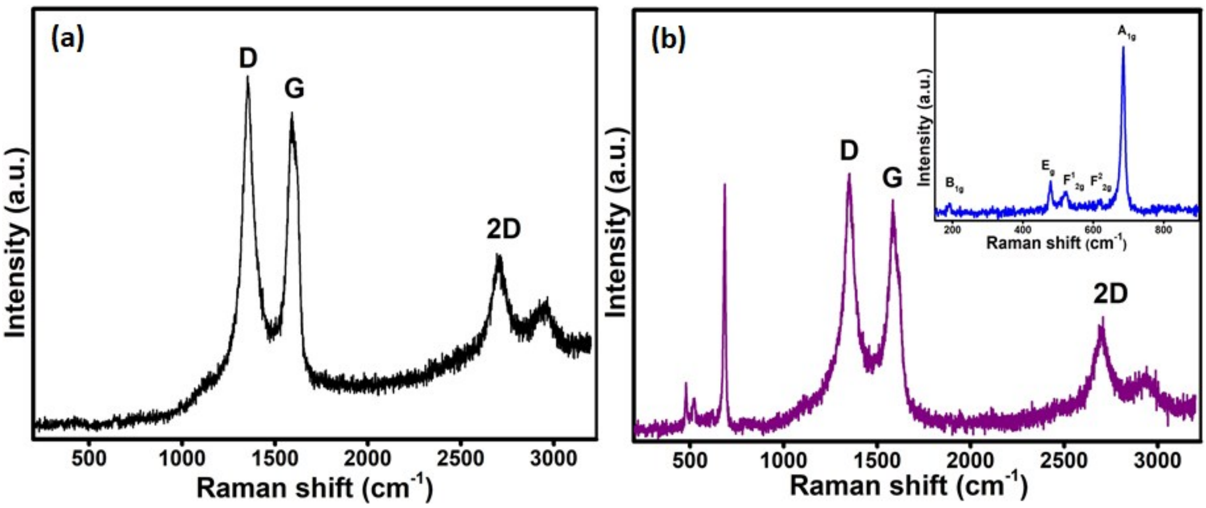

Figure S1 Raman spectrum of (a) acid treated MWCNTs and (b) Co_3O_4/Au@MWCNTs nanocomposite.

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