

Figures for the Supporting Information: Effect of Different Solvent Ratios (Water/Ethylene Glycol) on the Growth Process of CaMoO_4 Crystals and Their Optical Properties

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Figures for the Supporting Information

FIGURE SI-1:

Viscosity of different solvent ratios ($\text{H}_2\text{O}/\text{C}_2\text{H}_6\text{O}_2$) employed in preparation of CaMoO_4 crystals.

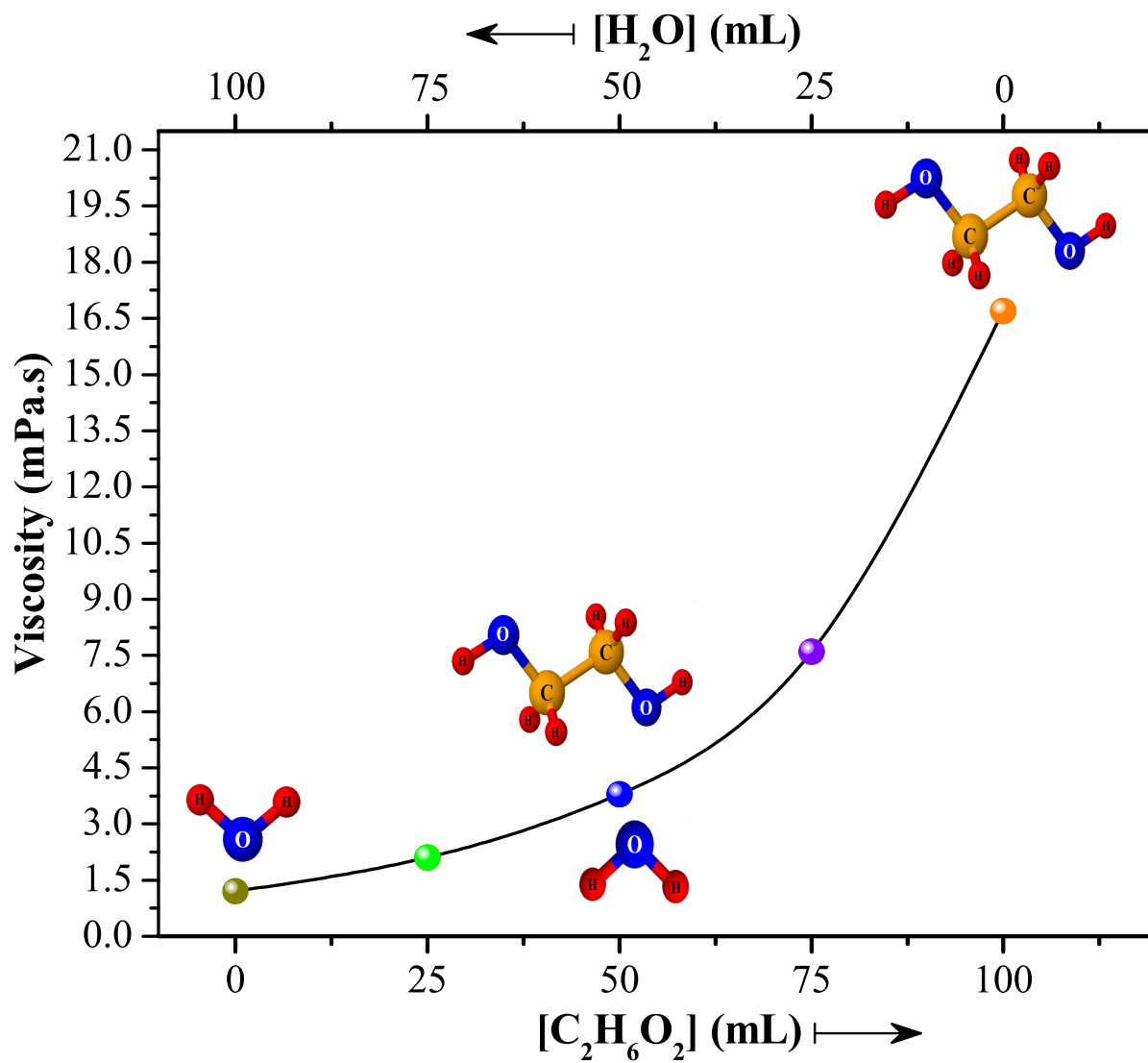


FIGURE SI-2:

Specific surface area of CaMoO_4 aggregated oriented crystals, meso and nanocrystals prepared with different solvent ratios ($\text{H}_2\text{O}/\text{C}_2\text{H}_6\text{O}_2$) and processed in microwave-assisted hydrothermal/solvothermal system at 140°C for 1 h.

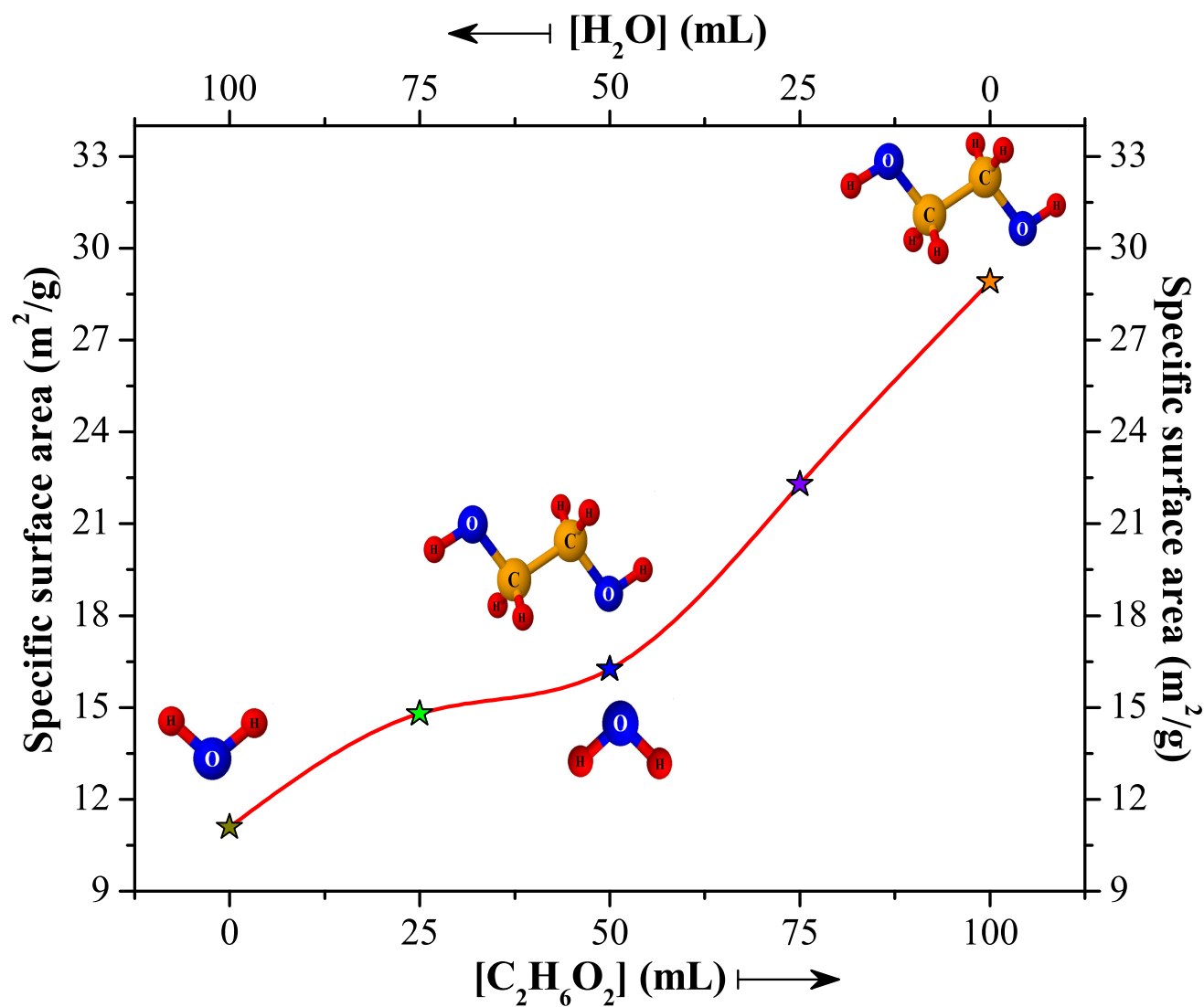


FIGURE SI-3(a-f):

N_2 adsorption-desorption isotherms of $CaMoO_4$ aggregated oriented crystals, meso and nanocrystals prepared with different solvent ratios ($H_2O/C_2H_6O_2$) and processed in microwave-assisted hydrothermal/solvothermal system at 140 °C for 1 h.

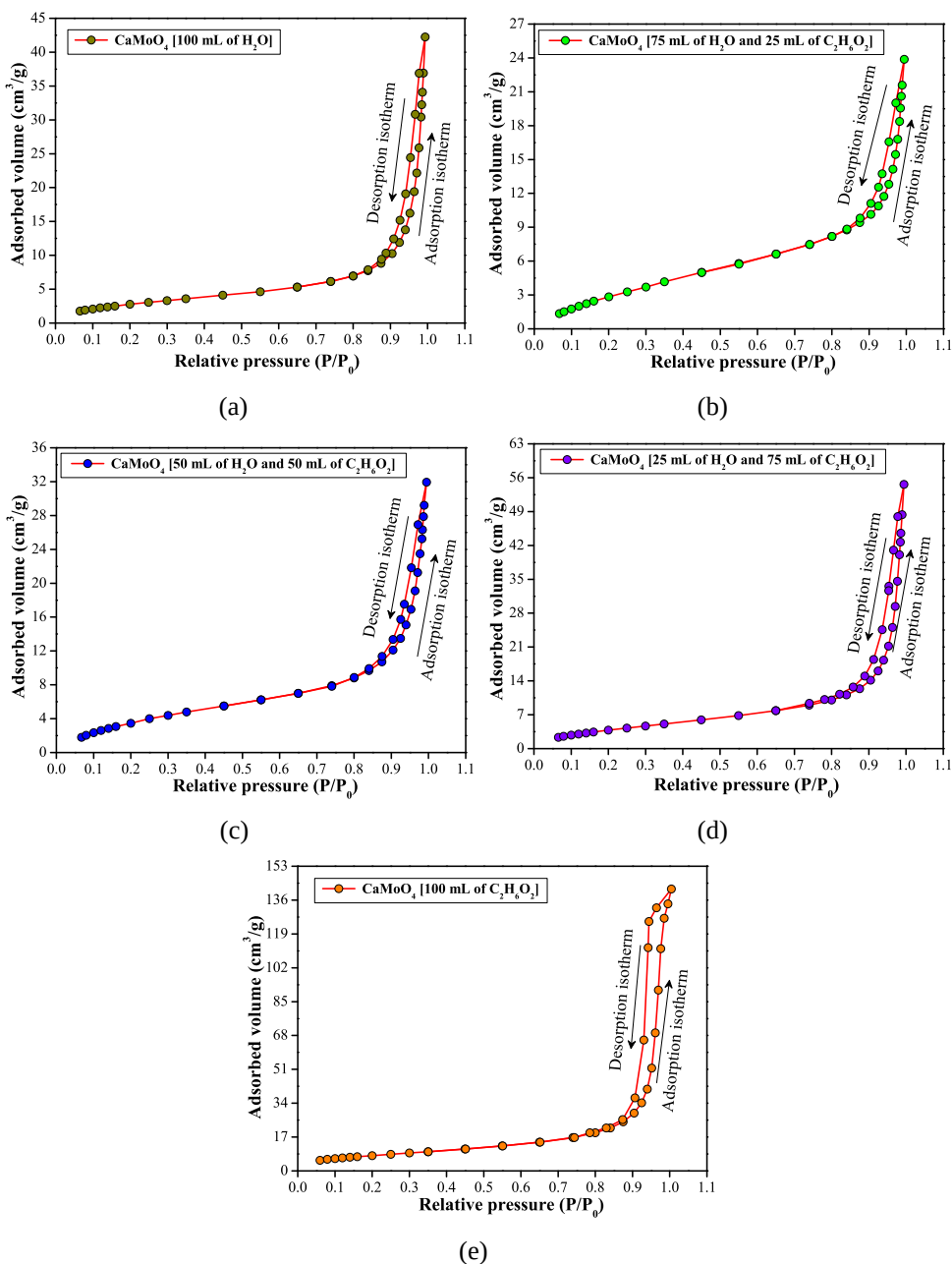


FIGURE SI-4(a-l):

TEM/HR-TEM micrographs and SAED of CaMoO_4 oriented aggregate crystals, meso and nanocrystals prepared with different solvent ratios and processed in microwave-assisted hydrothermal/solvothermal system: (a-d) 100 mL of H_2O , (e,f) 75 mL of H_2O and 25 mL of $\text{C}_2\text{H}_6\text{O}_2$, (g,h) 50 mL of H_2O and 50 mL of $\text{C}_2\text{H}_6\text{O}_2$, (i,j) 25 mL of H_2O and 75 mL of $\text{C}_2\text{H}_6\text{O}_2$ and (k,l) 100 mL of $\text{C}_2\text{H}_6\text{O}_2$.

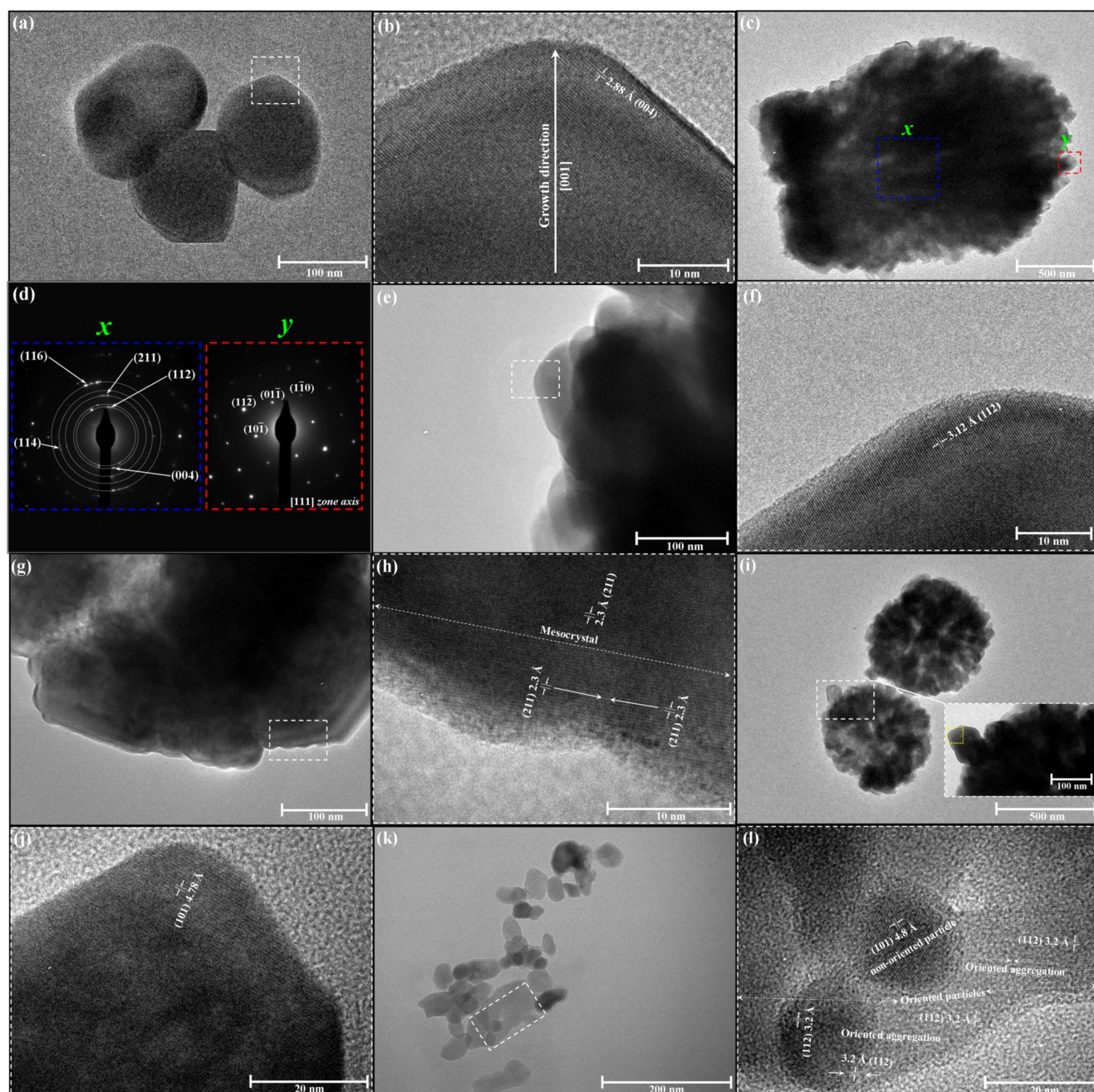


FIGURE SI-5(a-c):

Schematic representation of CaMoO_4 (a) oriented aggregate crystals, (b) meso and (c) nanocrystals and possible relation of orientation of crystals with the photoluminescence properties. Insets shows the digital photos of crystals exhibited photoluminescence at room temperature when excited by laser ($\lambda = 350 \text{ nm}$).

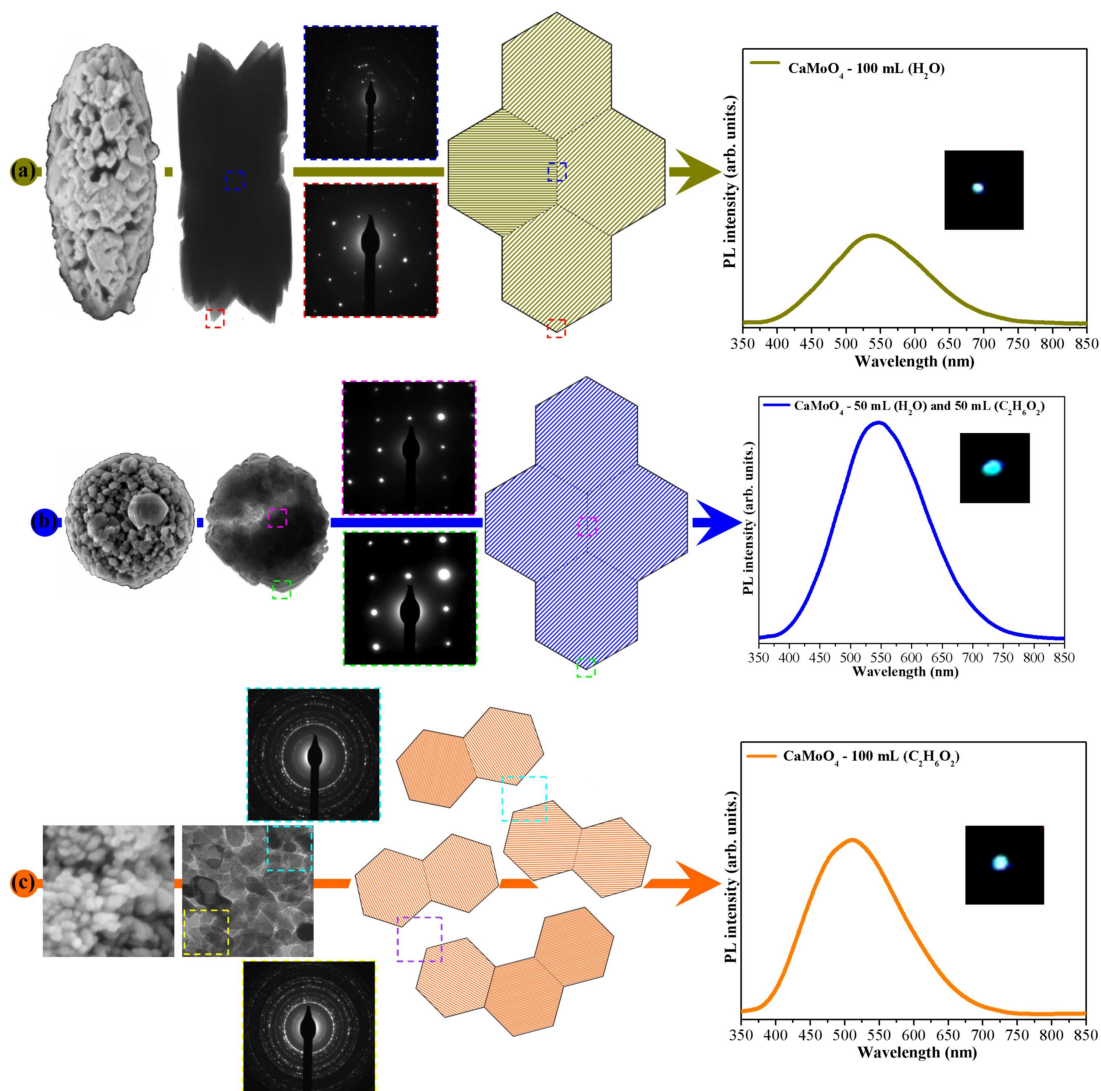


FIGURE SI-6:

Diagram of the primitive body-centered-tetragonal Brillouin zone.

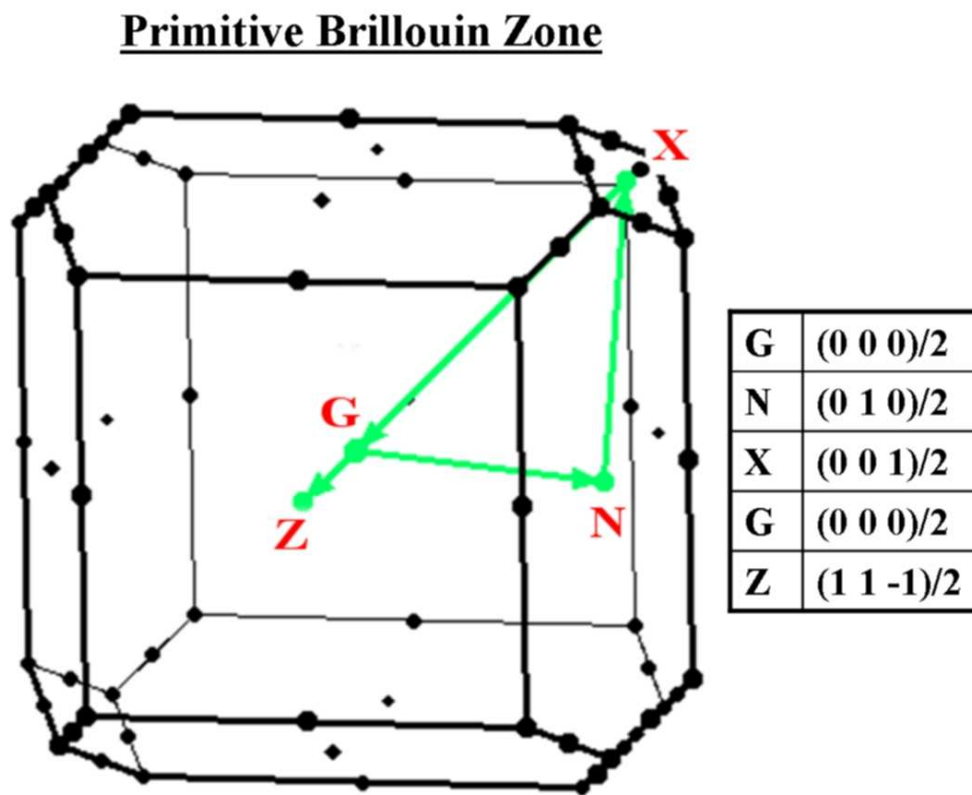


FIGURE SI-7:

Correlation of the experimental gap energy [$E_{gap(exp)}$] with the theoretical gap energy [$E_{gap(theo)}$] after the displacement of Mo atoms to deform the CaMoO_4 crystal.

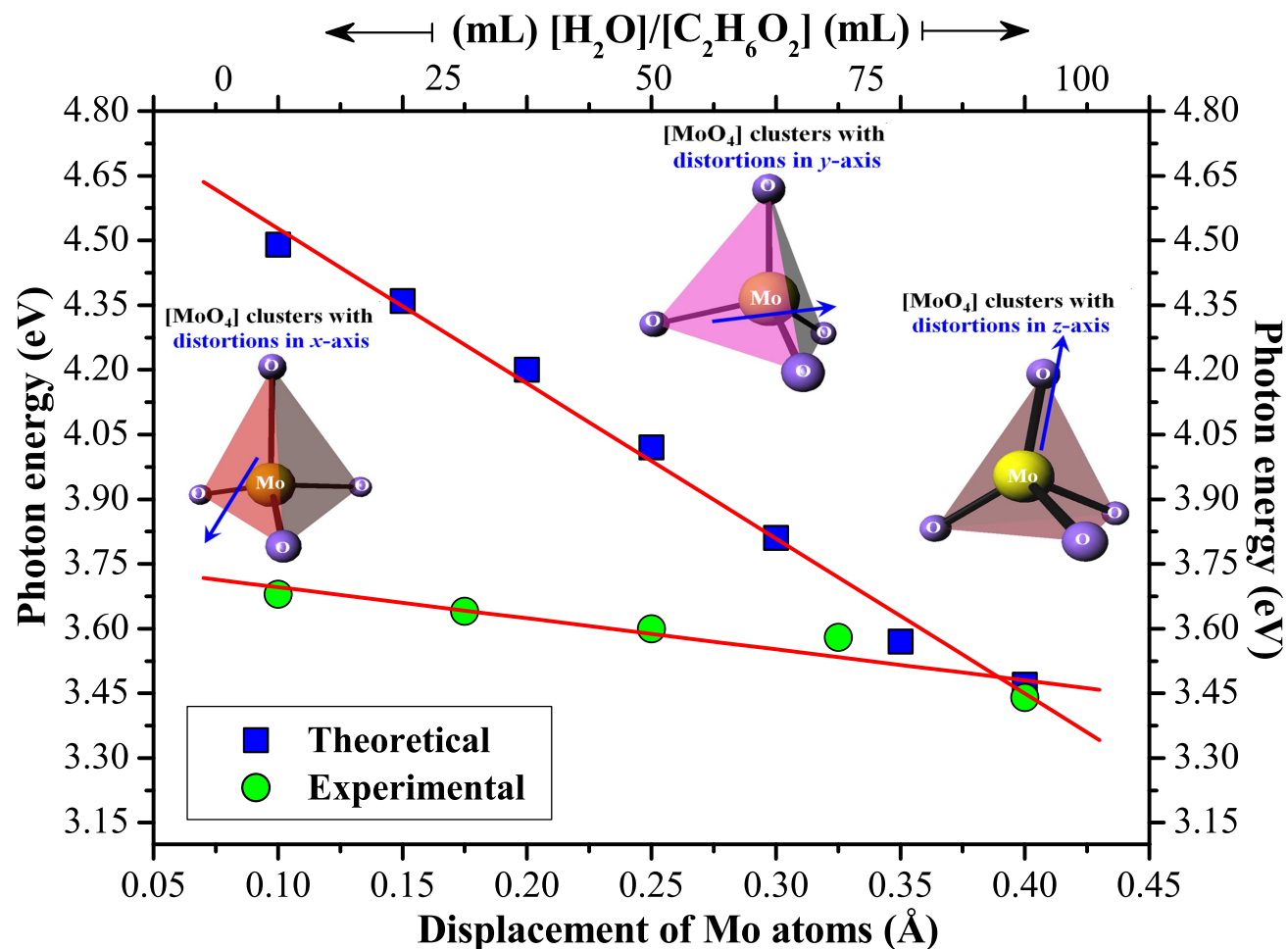


FIGURE SI-8:

DOS partial and total for each one of main atomics orbitals involved (Ca = 5s, 5p, O = 2p and Mo = 4d) of crystalline CaMoO_4 (a-c) without displacement on the Mo atoms.

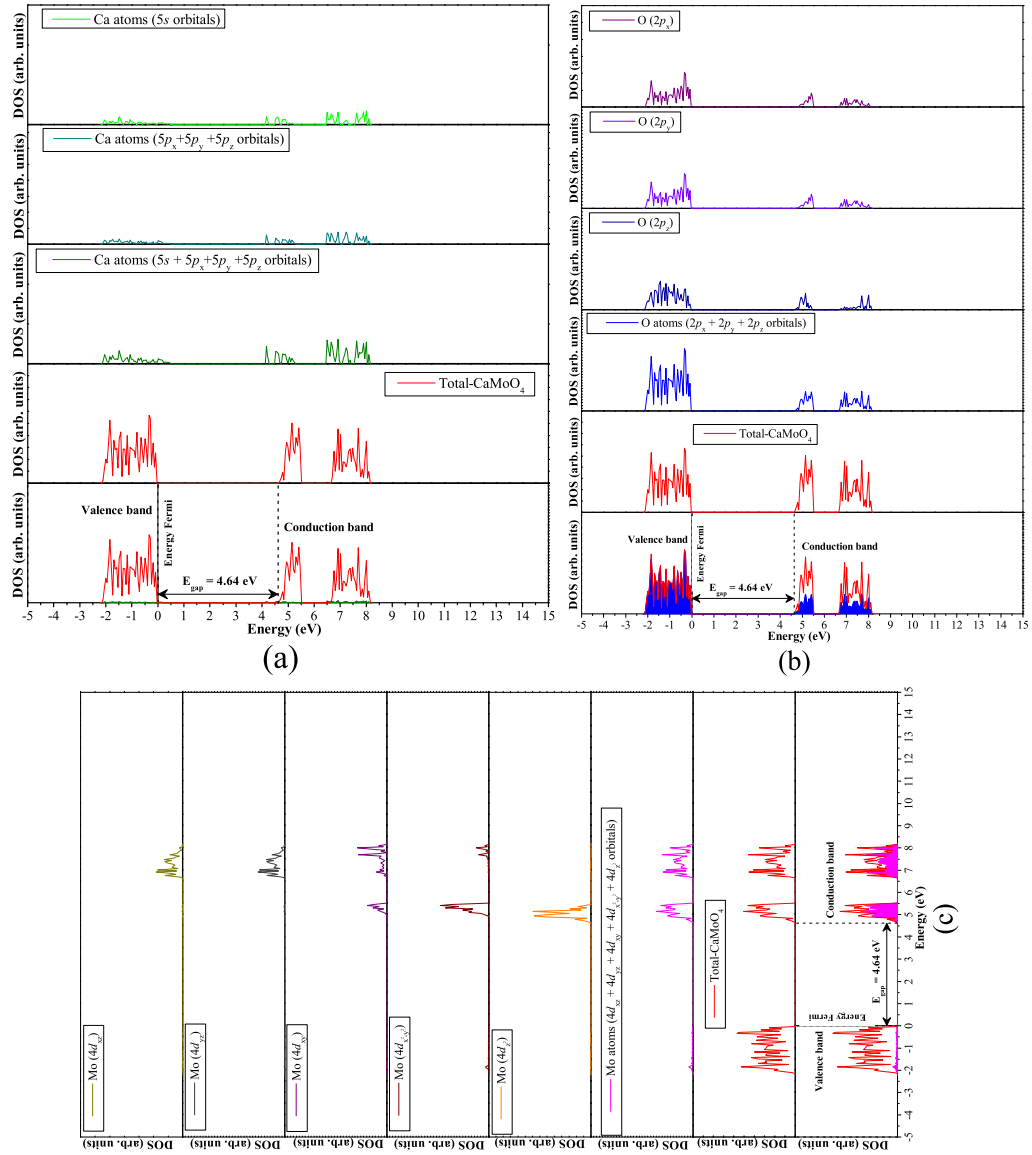


FIGURE SI-9:

DOS partial and total for each one of main atomics orbitals involved (Ca = 5s, 5p, O = 2p and Mo = 4d) of crystalline CaMoO_4 (a-c) with displacement of 0.35 Å on the Mo atoms.

