

Time- dependent DFT and experimental study on visible light photocatalysis by metal oxides of Ti, V and Zn after complexing with conjugated polymer

Navjot Kaur¹, Komal¹, Shuchi Gupta², Sonal Singhal^{1*} and Neetu Goel^{1*}

¹Department of Chemistry & Centre of Advanced Studies in Chemistry, Panjab University,
Chandigarh-160014, India

² University Institutes of Engineering and Technology, Panjab University, Chandigarh, 160014,
India

Supporting Information

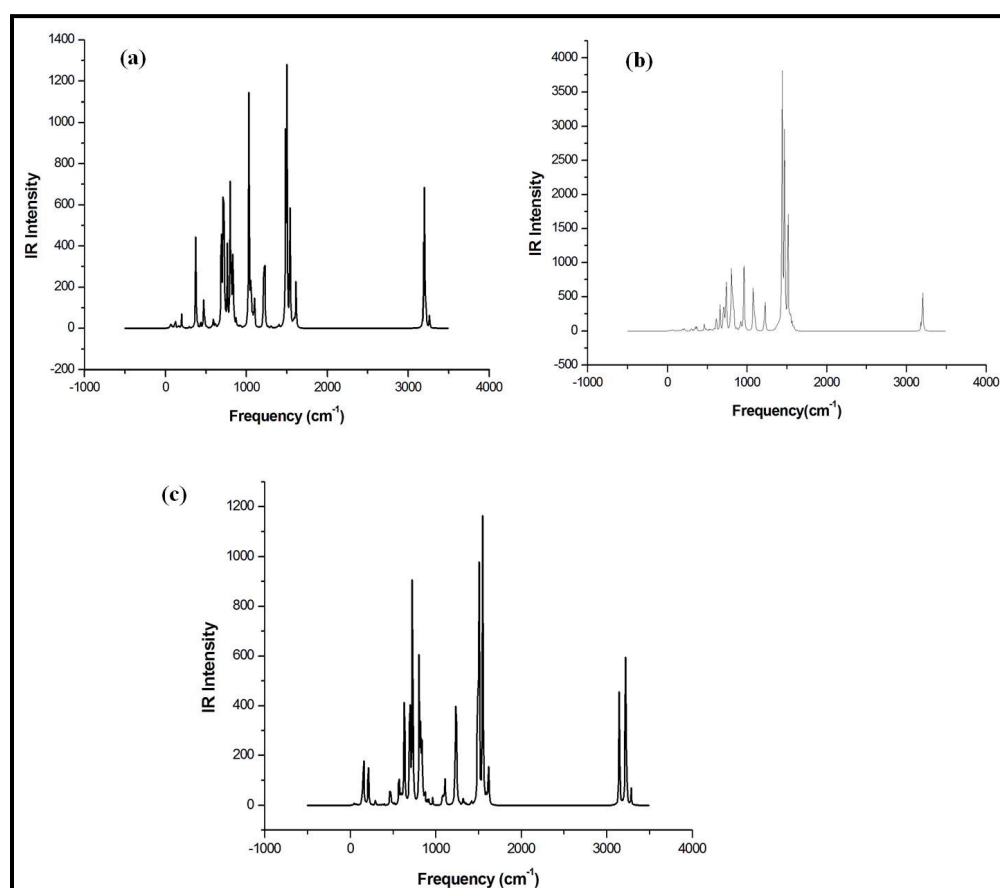


Figure S1. DFT calculated IR spectrum of (a) PTh-(TiO₂)₂ (b) PTh-V₂O₅ (c) PTh-(ZnO)₃ complexes.

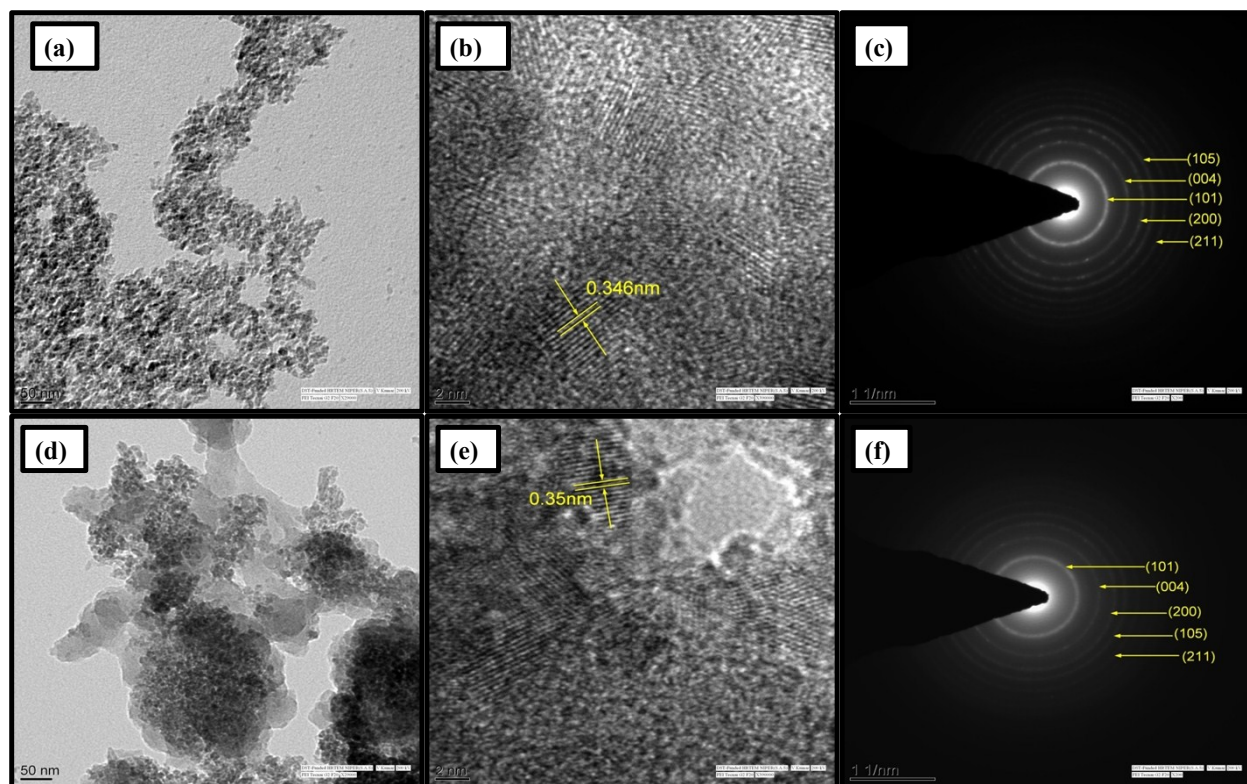


Figure S2. Low resolution TEM images (a and d), High resolution TEM images (b and e) and SAED pattern (c and f) for TiO₂ nanostructure and PTh-TiO₂ complex, respectively.

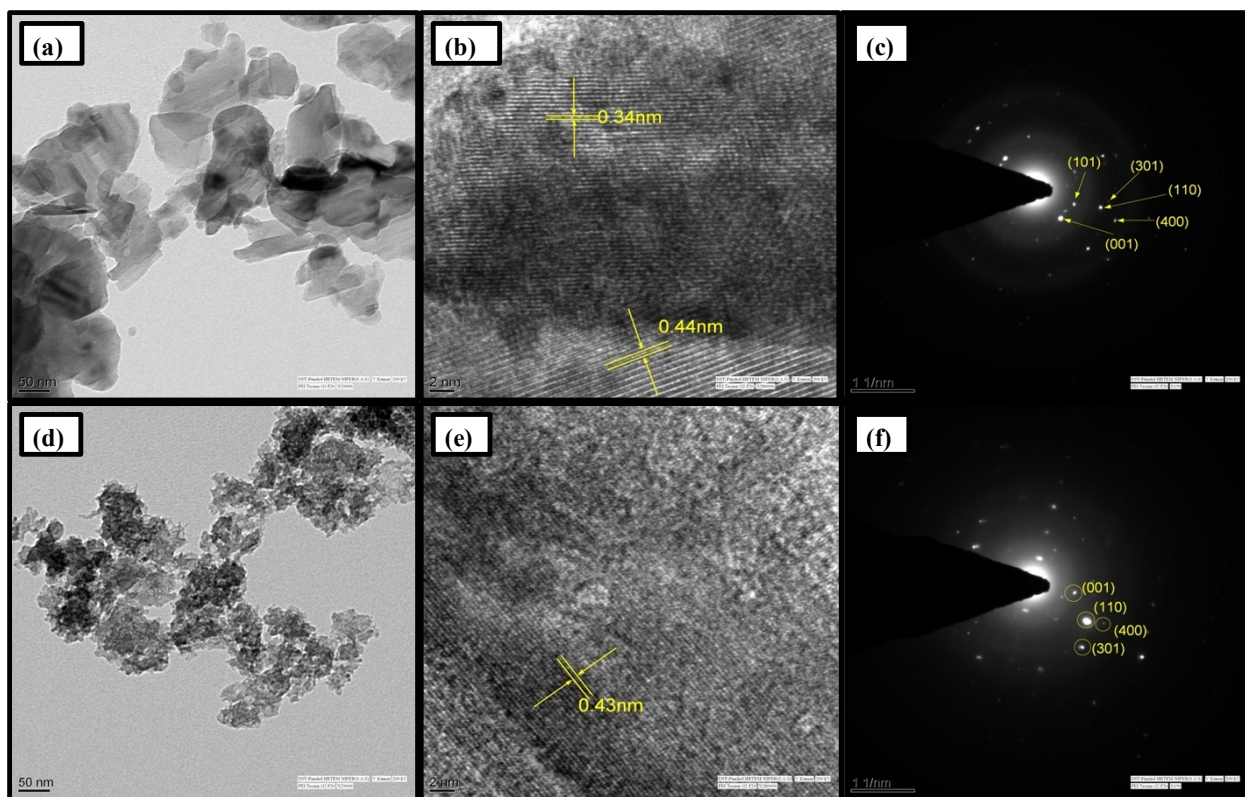


Figure S3. Low resolution TEM images (a and d), High resolution TEM images (b and e) and SAED pattern (c and f) for V_2O_5 nanostructure and PTh- V_2O_5 complex, respectively.

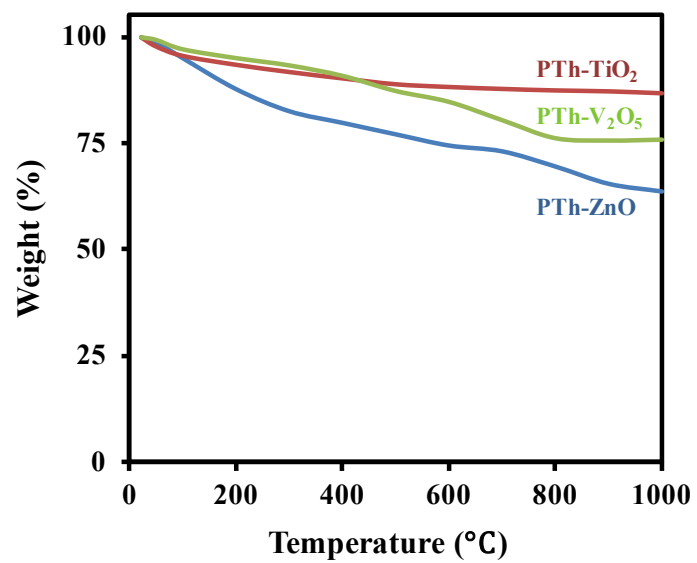


Figure S4. TGA thermograms of TMO-PTh nanocomposites.