



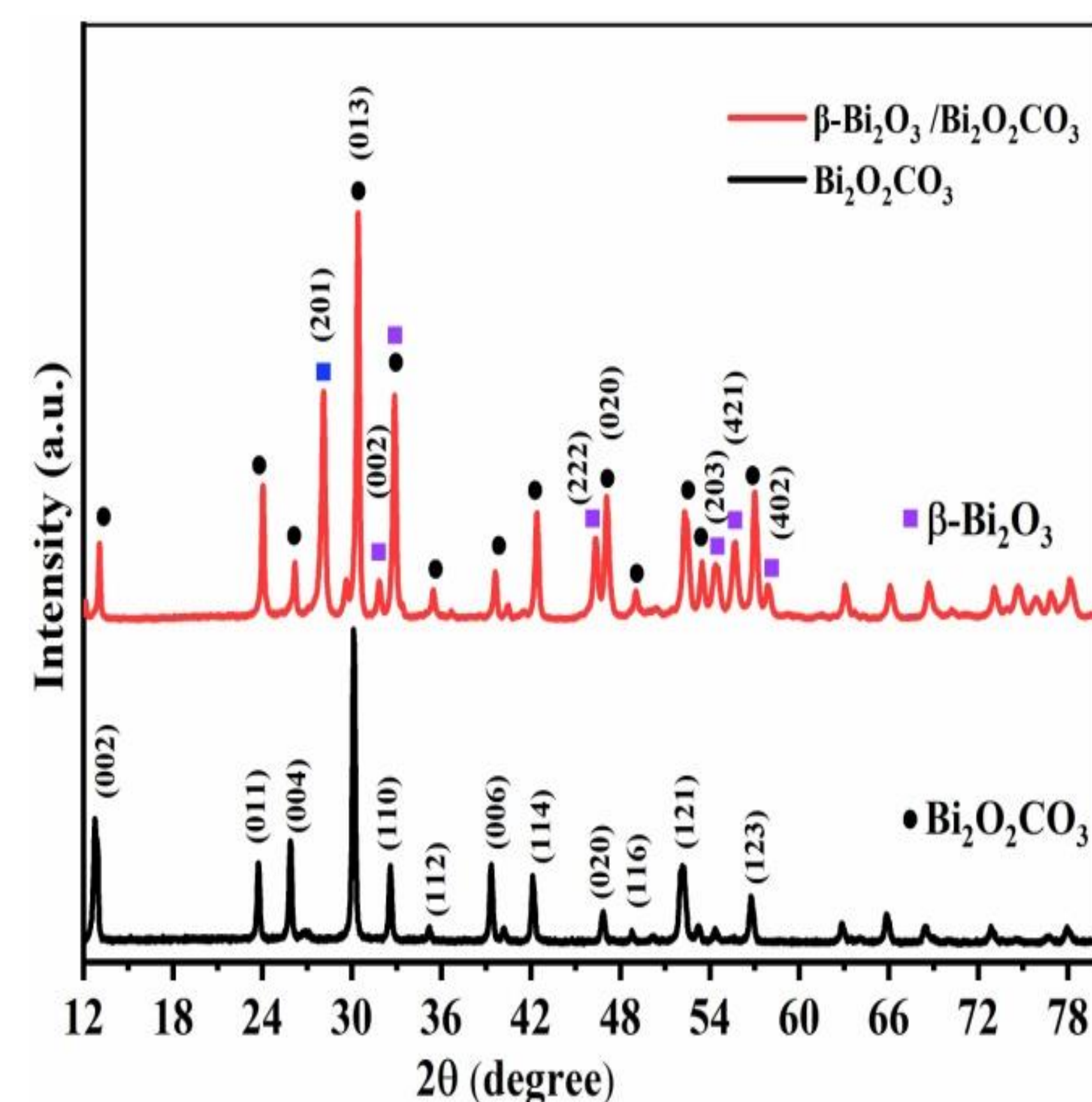
Adsorption of para-aminothiophenol on Non Noble Metaloxide Nanoparticles : A SERS and DFT Study

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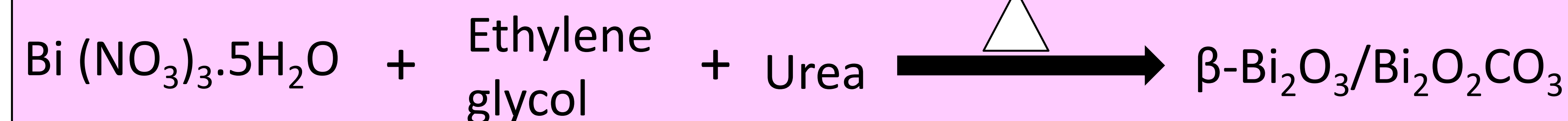
Introduction

- To obtain Genuine SERS spectra of PATP on noble metals has been a challenge.
- In this work using β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ nanoparticles a genuine SERS spectra of PATP was observed.

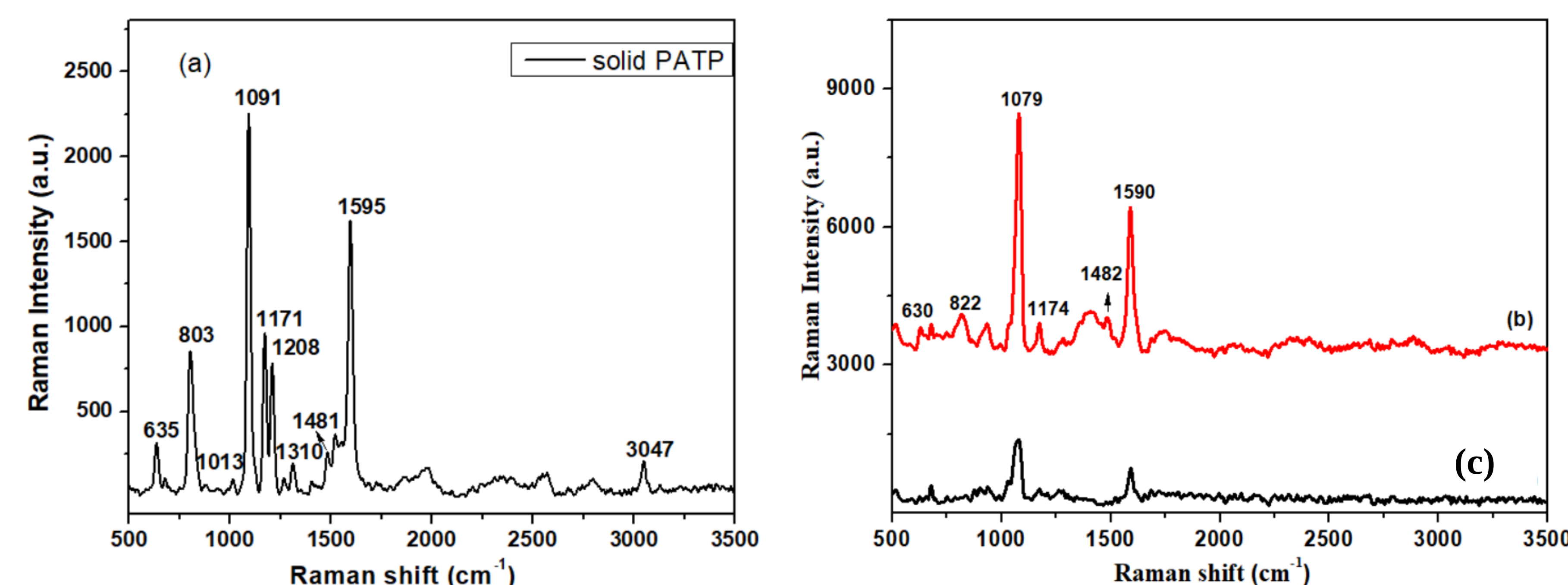


XRD Spectrum of β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ nanoparticles

Synthesis of β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ nanoparticles



Results



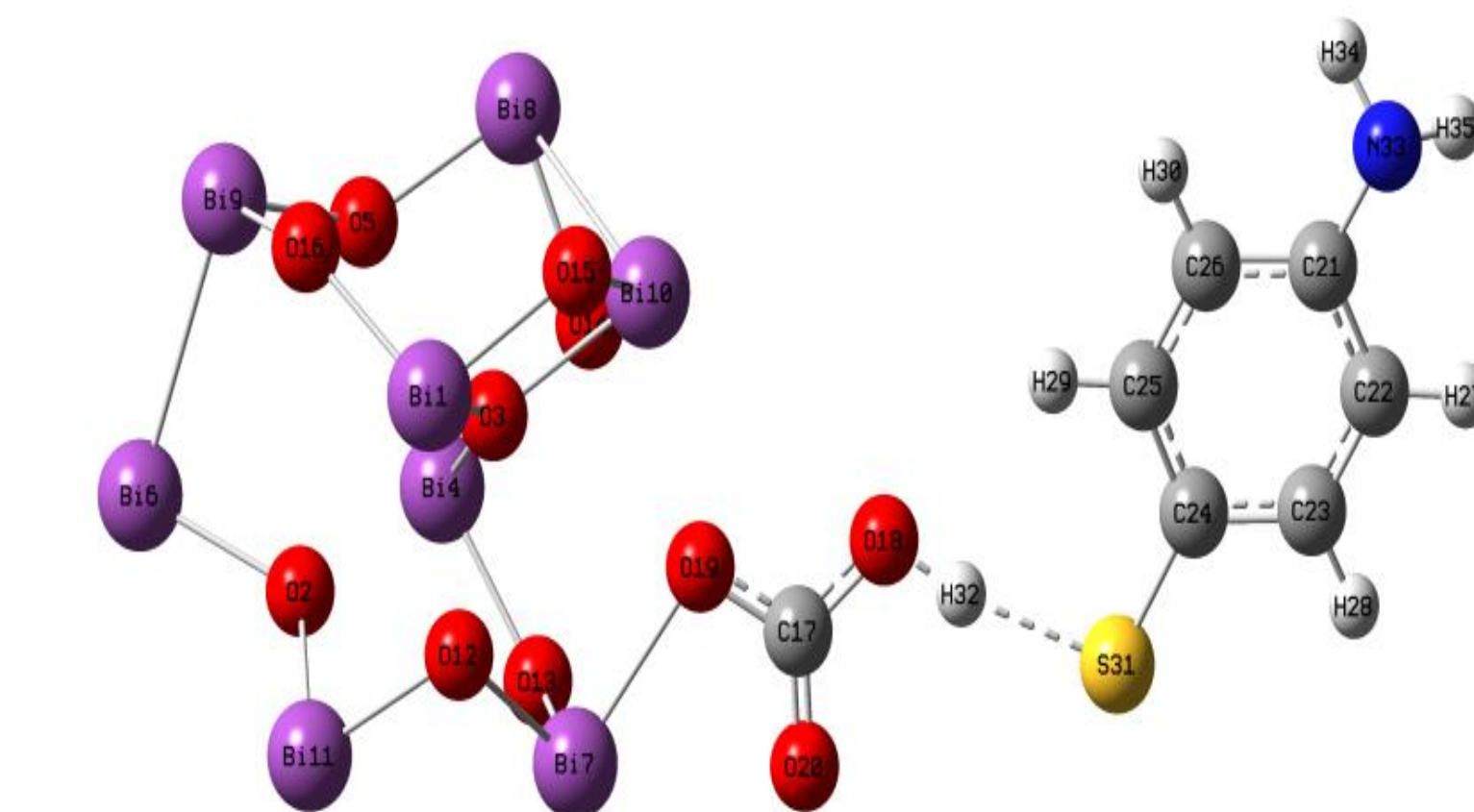
Raman spectrum of solid PATP (a), SERS spectrum of 10 mM PATP (b) and 5 mM PATP (c) on β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ nanoparticles

Conclusion

- The genuine SERS spectrum of PATP was observed which is in contrast to the case of noble metals.
- The simulated SERS spectrum of PATP-BOC are in good agreement with the one observed experimentally.
- The occurrence of genuine SERS spectrum of PATP on β - $\text{Bi}_2\text{O}_3/\text{Bi}_2\text{O}_2\text{CO}_3$ nanoparticles can be due to the charge transfer of PATP to BOC (Bismuthoxycarbonate) cluster.

Computational Method

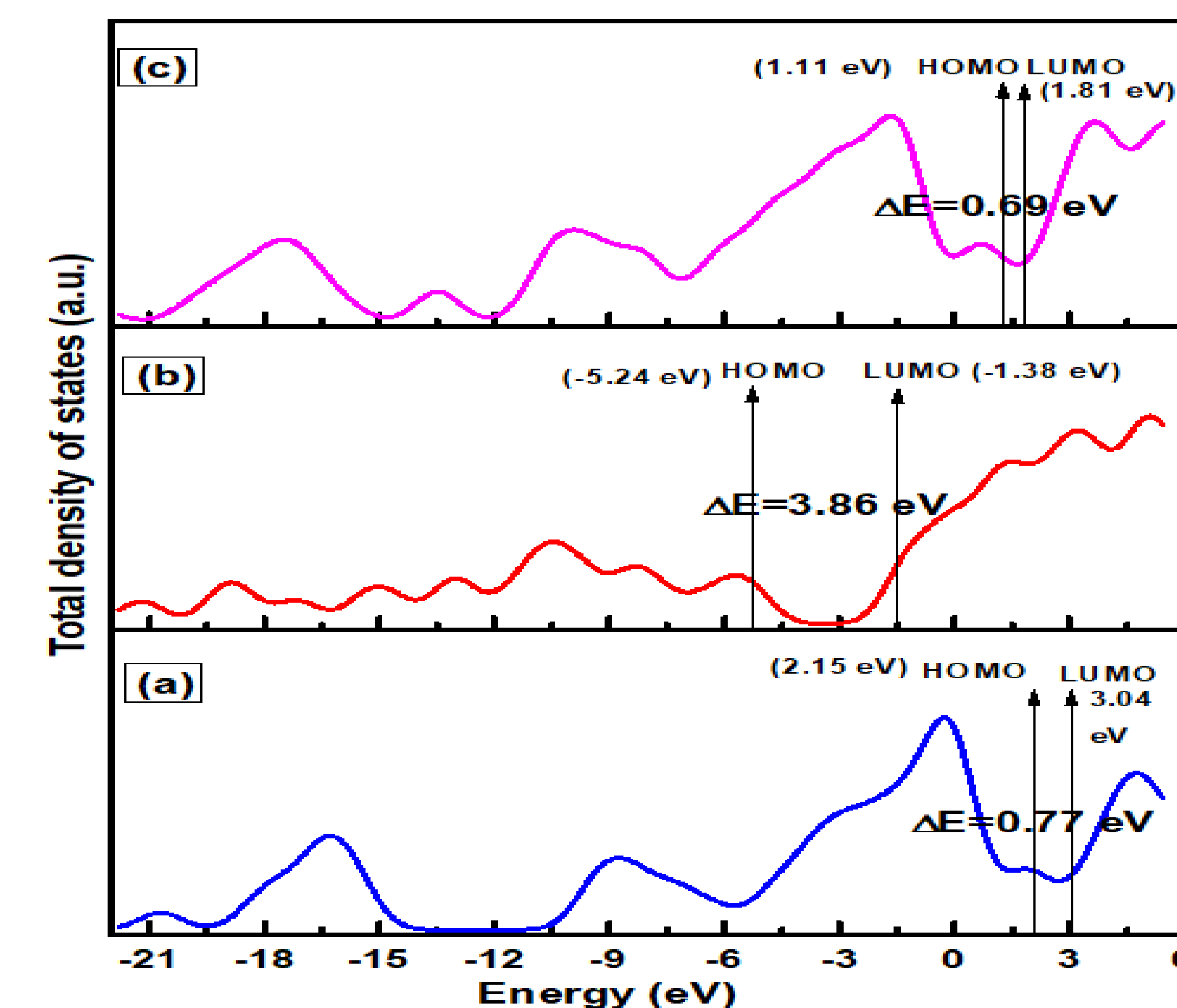
PW91PW91 functional and LANL2DZ basis set with relativistic effective core potential for Bi and 6-311+G(d,p) basis set for C,H,O,N and S atoms was utilized



Optimized structure of PATP-BOC with -54.87 kcal/mol interaction energy

Calculated and experimental SERS vibrational frequencies of PATP on BOC cluster at PW91PW91/LANL2DZ/6-311+G(d,p) level of theory

SERS peaks (cm ⁻¹)		Tentative Assignment#
Experimental	Calculated	
630	632	γ CCC
822	817.8	π CH
1079	1070.3	ν CS
1174	1157.7	δ CH
	1224	ν CN+ δ CH
1482	1458.3	ν CC+ γ CH
1590	1591.5	ν CC



Total density of plot of (a) BOC (Bismuthoxycarbonate) cluster (b) PATP and (c) PATP-BOC system showing energy of HOMO, LUMO and band gap (ΔE)

Acknowledgement

PARAM Shivay Facility under the National Supercomputing Mission, Government of India at the Indian Institute of Technology, Varanasi are gratefully acknowledged.