In-situ plasmon-driven chemical reactions revealed by high vacuum tip-enhanced Raman spectroscopy

Mengtao Sun,[1] Zhenglong Zhang,[1, 2] Hairong Zheng,[2] Hongxing Xu[1,*]

[1] Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P. O. Box 603-146, Beijing, 100190, People's Republic of China.

[2] College of Physics and Information Technology, Shaanxi Normal University, Xi'an, 710062, People's Republic of China.

Correspondence and requests for materials should be addressed to H.X.X. (email: hxxu@iphy.ac.cn).

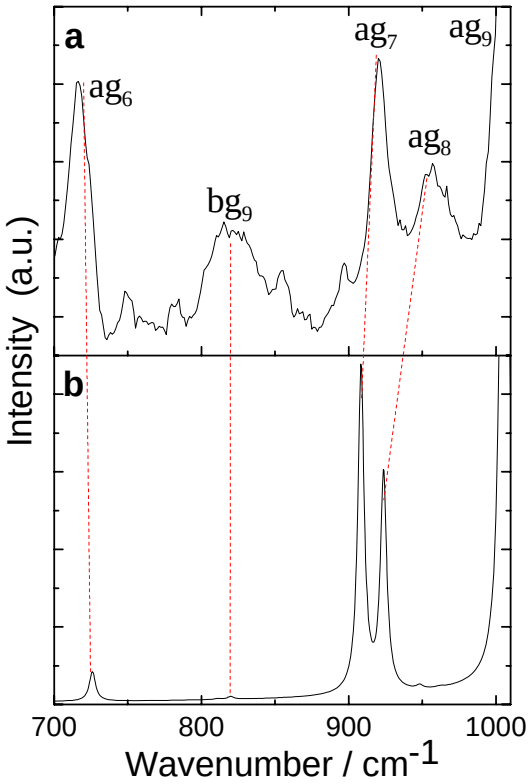


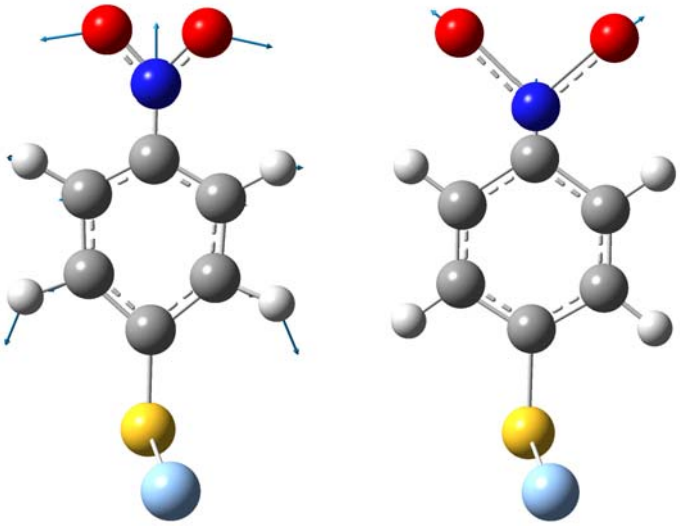
Figure. S1 (a) the TERS and (b) the simulated Raman spectrum of DMAB at low frequencies.

Theoretical simulations. To assign these Raman peaks in Fig. 2, the quantum chemical calculations on Raman spectra of DMAB were done with density functional theory (DFT),[a] PW91 functional and TZP basis set, using ADF suite.[b]

References:

[a]. Dreizler, M.R., Gross, E. K.U.Density Functional Theory, Springer-Verlag, Heidelberg, 1990.

[b]. Amsterdam Density Functional, version 2011, www.scm.com.



854cm^{-1} 1336 cm^{-1}

Figure. S2. The vibrational modes of 4NBT adsorbed on Ag at 854 cm^{-1} (bending) and 1336 cm^{-1} (stretching), respectively.

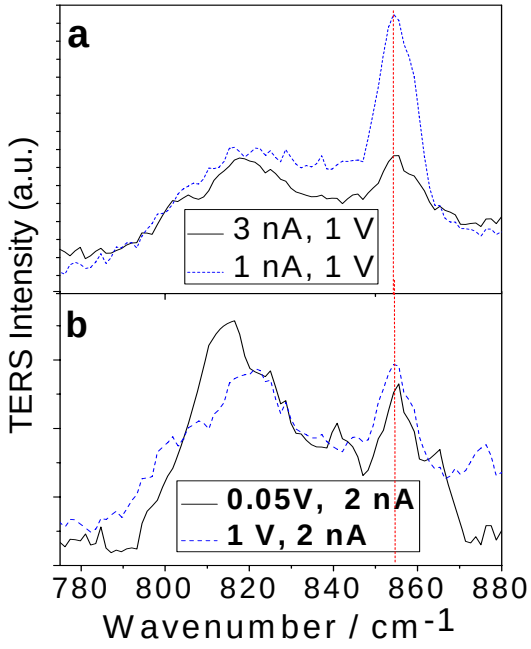


Figure. S3 (a) current and (b) voltage dependent TERS spectra of DMAB around 854 cm^{-1} for -NO2 bending vibrational mode of 4NBT.