Multitasking Behaviour of a Small Organic Compound: Solid State Bright White-Light Emission, Mechanochromism and Ratiometric Sensing of Al(III) and Pyrophosphate

Sanghamitra Sinha, [†] Bijit Chowdhury, [†] Uttam Kumar Ghorai[#] and Pradyut Ghosh*[†]

[†]School of Chemical Sciences, Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Kolkata 700 032, India.

[#]Department of Industrial Chemistry and Applied Chemistry, Ramakrishna Mission Vidyamandira & Swami Vivekananda Research Center, Belur Math, India

| Contents | Page no. |
|---|-------------|
| 1. Experimental Section | S2 |
| 2. Scheme S1. Synthesis of 1H | S4 |
| 3. Figure S1-S7. Characterization of 1H | S4-S7 |
| 4. Figure S8-S11 & Table S1. Crystallographic data of 1H | S8-S10 |
| 5. Figure S12. TGA and DSC of 1H | S11 |
| 6. Figure S13. Solid state Excitation | S11 |
| 7. Figure S14. Solid state TCSPC | S12 |
| 8. Figure S15. Mechanochromic behavior of 1H | S12 |
| 9. Figure S16. TGA and DSC of 1H after grinding | S13 |
| 10. Figure S17. PXRD data and mechanochromic reversibility | S 13 |
| 11. Figure S18. UV-PL spectra of 1H | S14 |
| 12. Scheme S2 & Figure S19-S20. Synthesis and characterization a of 1Me | S14-S15 |
| 13. Figure S21. UV-PL spectra of 1Me in acetonitrile | S16 |
| 14. Figure S22. PL spectra of 1H and 1Me in different solvents | S16 |
| 15. Figure S23. Solid state photophysical studies of 1Me | S17 |
| 16. Figure S24-S26. Microscopic studies; AFM and DLS data | S18-S19 |
| 17. Figure S27-S34, Table S2, S3. Sensing studies of 1H and 1Me | S19-S24 |

Experimental Section:

Materials. The reactions and workup procedures were performed at ambient condition. 9,10phenanthrenequinone, ammonium acetate and Glacial acetic acid were purchased from Spectrochem Pvt. Ltd., India; 2-hydroxy-1-naphthaldehyde and 2-methoxy-1-naphthaldehyde were purchased from Alfa Aesar. Perchlorate salt of metals and tert-butylammonium salt of PPi were obtained from Aldrich and were used as received. HPLC-grade solvents and doubly distilled water were used in spectral measurements. NMR solvent DMSO- d_6 was purchased from Aldrich.

Methods. ¹H, ¹³C, ¹H-¹H COSY, ¹H-DEPT-135 HSQC and ¹H-¹³C HMBC NMR experiments were carried out on FT-NMR Bruker DPX 300/400/500 MHz NMR spectrometer, and the chemical shift values for ¹H and ¹³C NMR were reported in parts per million (ppm), calibrated to the residual solvent peak set. High-resolution mass spectrometry (HRMS) analyses were done by QTOF-Micro YA 263 mass spectrometer in positive ESI mode. Fourier transform infrared (FTIR) spectra were recorded on Shimadzu FTIR-8400S infrared spectrophotometer with KBr pellets. Elemental analysis was performed on PerkinElmer 2500 series II elemental analyzer, Perkin Elmer, USA. The UV-vis absorption spectrum was obtained using Perkin Elmer Lambda 950. The solid-state photoluminescence spectra and corresponding CIE diagrams were obtained using an FLS980 spectrofluorimeter (Edinburgh Instruments) and a 450 W xenon lamp as the light source under ambient conditions. An inbuilt filter was present in the fluorimeter to avoid the appearance of the second order harmonic peak. Time-correlated single photon count measurement to determine the lifetime was measured using a 275 nm picosecond pulsed LED and an MCP detector. Solution phase emission spectra were recorded in a FluoroMax-3 spectrophotometer, from Horiba Jobin Yvon.

Caution! Metal perchlorate salts are explosive in the presence of open flames, heat or sparks. Aluminum perchlorate is a skin irritant. All due precautions should be taken to handle these.



Chart S1. Molecular structure of 1H.

Synthesis of 1-(1H-phenanthro[9,10-d]imidazol-2-yl)naphthalen-2-ol (1H). A solution of 9,10-phenanthrenequinone (0.250 g, 1.2 mmol), 2-hydroxy-1-naphthaldehyde (0.206 g, 1.2 mmol), and ammonium acetate (1.5 g, 19.5 mmol) in glacial acetic acid (8 mL) was stirred at 90 °C for 3 h. The reaction mixture was then poured into ice-cold water. Resulting precipitate was filtered, washed properly with water, and dried in air. The cream-white residue was purified by medium-pressure column chromatography with silica gel of 60-120 mesh size using ethyl acetate/ petroleum ether as the eluent. Pure product was isolated at 15% ethyl acetate concentration as white powder (0.30 g, 70%). Elemental analysis: Calcd (%) for C₂₅H₁₆N₂O: C, 83.31; H, 4.47; N, 7.77; O, 4.44. Found: C, 83.39; H, 4.40; N, 7.85. FTIR in KBr disc (v/cm⁻¹): 3446, 3049, 2921, 2924, 2850, 2363, 1620, 1466, 1331, 1248, 816, 749. ESI-MS $[C_{25}H_{16}N_2O][H^+]$ calcd: m/z 361.41. Found: m/z 361.09. ¹H NMR (500 MHz, DMSO-*d*₆, Si(CH₃)₄): δ 13.36 (bs, 1H, OH), 10.93 (bs, 1H, NH), 8.89 (d, J = 10 Hz, 2H, H_{g,g'}), 8.53 (d, J =

10 Hz, 2H, H_{d,d'}), 7.98 (d, J = 5 Hz, 2H, H_{s,c}), 7.92 (d, J = 10 Hz, 1H, H_b), 7.72 (t, J = 15 Hz, 2H, H_{e,e'}), 7.64 (t, J = 15 Hz, 2H, H_{f,f'}), 7.48 (t, J = 15 Hz, 1H, H_i), 7.37 (t, J = 15 Hz, 2H, H_{h,a}). ¹³C NMR (100 MHz, DMSO- d_6 , Si(CH₃)₄): δ 154.7 (1C, C_k), 146.2 (1C, C_m), 132.9 (1C, C₁), 131.1(1C, C_s), 128.0 (1C, C_b), 127.8, 127.4, 127.0 (3C, C_{i,e,e'}), 125.0 (2C, C_{f,f'}), 124.2 (1C, C_c), 123.8 (2C, C_{g,g'}), 123.1 (1C, C_a), 121.8 (2C, C_{d,d'}), 118.3 (1C, C_h), 110.1 (1C, C_i).



Scheme S1. Synthetic scheme for 1H.



Figure S1. ¹H-NMR (500 MHz) spectrum of 1H in DMSO- d_6 .



Figure S2. 1 H- 1 H COSY-NMR (500 MHz) spectrum of 1H in DMSO- d_{6} .



Figure S3. ¹³C-NMR (125 MHz) spectrum of 1H in DMSO- d_6 .



Figure S4. DEPT-135-NMR (125 MHz) spectrum of 1H in DMSO-*d*₆.



Figure S5. ¹H-DEPT-135 HSQC-NMR (500 MHz) spectrum of 1H in DMSO-*d*₆.



Figure S6. 1 H- 13 C-HMBC NMR (500 MHz) spectrum of 1H in DMSO- d_{6} .



Figure S7. ESI-MS of 1H.

X-ray Crystallographic Refinement Details for 1H. The crystals of **1**H were obtained from slow evaporation of the compound in DMSO. Fromthere, a diffractable size crystal was collected, dipped in paratone oil, and then was cemented on the tip of a glass fiber using epoxy resin. Intensity data of the crystal were collected using Mo K α ($\lambda = 0.7107$ Å) radiation on a Bruker SMART APEX diffractometer, equipped with a CCD area detector at 293K. Data integration and reduction were processed by SAINT¹ software. Empirical absorption correction to the collected reflections was done by applying SADABS.² The structure was solved using SHELXTL³ and was refined on F² by the full-matrix least-squares technique using the SHELXL-97⁴ program package. PLATON-97⁵ and MERCURY 3.8⁶ were used to generate graphics. CCDC-1857506 contains the supplementary crystallographic data for this paper. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.



Figure S8. Single-crystal X-ray structure of **1**H (thermal ellipsoids are drawn at 60% probability level) showing the asymmetric unit. Color code: O, red; N, blue; C, gray; H, pink.

| Compound reference | 1 H | Space group | P2(1)/n |
|---------------------|-----------------------|---------------------------------------|---------|
| Chemical formula | $C_{27}H_{22}N_2O_2S$ | No. of formula units per unit cell, Z | 4 |
| Formula Mass | 438.53 | Radiation type | ΜοΚα |
| Crystal system | Monoclinic | Absorption coefficient, μ /mm-1 | 0.160 |
| a/Å | 6.8651(5) | No. of reflections measured | 22865 |
| b/Å | 19.3795(13) | No. of independent reflections | 4228 |
| c/Å | 18.3270(13) | R _{int} | 0.0615 |
| α/° | 90.00 | Final R1 values (I > $2\sigma(I)$) | 0.0669 |
| β/° | 99.218(2) | Final wR(F2) values (all data) | 0.1858 |
| γ/° | 90.00 | Goodness of fit on F2 | 1.219 |
| Unit cell volume/Å3 | 2406.8(3) | CCDC | 1857506 |
| Temperature/K | 293(2) | | |

 Table S1. Crystallographic parameter details of 1H.



Figure S9. Three-dimensional crystal packing of **1**H illustrating the layered array of molecules connected *via* intermolecular interactions; Color code: O, red; N, blue; C, gray; H, white.



Figure S10. A slice of three-dimensional (3-D) crystal packing of **1**H along the crystallographic *a* axis showing intermolecular stacking (thermal ellipsoids are drawn at 60% probability level). Color code: O, red; N, blue; C, gray (H atoms are omitted for clarity).



Figure S11. A slice of three-dimensional (3-D) crystal packing of 1H along the crystallographic *b* axis (thermal ellipsoids are drawn at 60% probability level). Color code: O, red; N, blue; C, gray (H atoms are omitted for clarity).



Figure S12. (a) Thermo-gravimetric and (b) differential scanning calorimetric analysis of 1H.



Figure S13. Solid state excitation spectrum of 1H (a) before ($\lambda_{em} = 580$ nm) and (b) after grinding ($\lambda_{ex} = 475$ nm).

Quantum yield calculation. The PL quantum yield (Φ_f) was calculated using an analytical approach following the equation given below.⁷

$$\Phi_{f} = \frac{\int_{\lambda_{\rm em_{1}}}^{\lambda_{\rm em_{2}}} \frac{\left[I_{\rm x}(\lambda_{\rm em}) - I_{\rm b}(\lambda_{\rm em})\right]}{s(\lambda_{\rm em})} \lambda_{\rm em} d\lambda_{\rm em}}{\int_{\lambda_{\rm ex} - \Delta\lambda}^{\lambda_{\rm ex} + \Delta\lambda} \frac{\left[I_{\rm b}(\lambda_{\rm ex}) - I_{\rm x}(\lambda_{\rm ex})\right]}{s(\lambda_{\rm ex})} \lambda_{\rm ex} d\lambda_{\rm ex}} = \frac{N_{\rm em}}{N_{\rm abs}}$$

where, the total number of emitted photons (N_{em}) is obtained upon integration of the blankcorrected $(I_b(\lambda_{em}))$ and spectrally corrected $(I_x(\lambda_{em}))$ emission spectrum of the sample. The number of absorbed photons (N_{abs}) follows from the integrated difference between the excitation light resulting from measurements with the blank $(I_b(\lambda_{ex}))$ and the sample $(I_x(\lambda_{em}))$. $s(\lambda_{em})$ and $s(\lambda_{ex})$ are spectral responsivity of the emission and excitation channel respectively.



Figure S14. Fluorescence decay profiles of **1**H monitored at 470 and 580 nm (a) before and (b) after grinding.



Figure S15. Change in emission color of **1**H during application of mechanical pressure and its regeneration by heating.



Figure S16. (a) Thermo-gravimetric and (b) differential scanning calorimetric analysis of **1**H after grinding.



Figure S17. (a) Change in PXRD pattern of **1**H during application of mechanical pressure and its regeneration by heating; (b) change in PXRD pattern of **1**H during its regeneration from the grinded form by applying heat; (c) change in I580/I475 value of **1**H with repetitive cycles of grinding and heating at 65°C for 4h.



Figure S18. Absorption and emission spectral behavior of 1H.

Synthesis of 2-(2-Methoxyphenyl)-1H-phenanthro[9,10-d]- imidazole (1Me). A solution of 9,10-phenanthrenequinone (0.250 g, 1.2 mmol), 2-methoxybenzaldehyde (0.223 g, 1.2 mmol), and ammonium acetate (1.5 g, 19.5 mmol) in glacial acetic acid (8 mL) was stirred at 90 °C for 4 h. The reaction mixture was poured into ice-cold water. Resulting precipitate was filtered, washed properly with water, and dried. Pure product was obtained as brownish white powder. (0.382 g, 85%). Elemental analysis: Calcd (%) for $C_{22}H_{16}N_2O$: C, 81.46; H, 4.97; N, 8.64; O, 4.93. Found: C, 81.22; H, 5.13; N, 8.31; O, 4.65. ESI-MS [$C_{26}H_{18}N_2O$][H⁺] calcd: m/z 375.43. Found: m/z 375.00. ¹H NMR (500 MHz, DMSO- d_6 , Si(CH₃)₄): 13.47 (s, 1H), 8.92-8.87 (m, 2H), 8.55 (d, J = 8 Hz, 1H), 8.40 (d, J = 8 Hz, 1H), 8.19 (d, J = 8 Hz, 1H), 8.00 (d, J = 8 Hz, 1H), 7.74-7.70 (t, J = 16 Hz, 3H), 7.69-7.65 (t, J = 16 Hz, 3H), 7.46-7.42 (m, 2H), 3.93 (s, 3H).



Scheme S2. Synthetic scheme for 1Me.



Figure S19. ¹H-NMR (400 MHz) spectrum of 1Me in DMSO-*d*₆.



Figure S20. ESI-MS of 1Me.



Figure S21. Absorption and emission spectral behavior of 1Me.



Figure S22. Emission spectra of **1**H and **1**Me in solvents of different polarity ($\lambda_{ex} = 360$ nm).

Solvent polarity dependent photoluminescence studies of **1**H does not show any well shifted emission bands for enol and keto forms, even in aprotic nonpolar solvents like hexane, toluene etc., which is commonly observed in case of ESIPT based systems. Both **1**H and **1**Me display shift in the wavelength of higher energy emission band, while, the position of the lower energy emission band does not change significantly (Fig. S22, ESI[†]). The results suggest that the higher

energy emission band (~ 460 nm) might be originated from the locally excited state (LE), while, the lower energy emission (~ 420 nm) could arise from the excited state intramolecular charge transfer (ESICT) process⁸ which is occurring in both the systems. The extent of ESICT is less in 1Me. However, the steric repulsion between the imidazole NH group and the nearby naphthyl CH part might cause difficulty for 1H to adopt planar geometry which is needed for ESIPT to happen and that is why the molecule does not show ESIPT process even in solution.

36. ESIPT is a fast (picosecond) intramolecular proton-transfer process, occurs in excited state of suitable molecules containing -OH/-NH and C=N/C=O, etc. functionalities, which results large Stokes shift.



Figure S23. Solid state emission spectral change of 1Me upon grinding, with corresponding CIE diagrams ($\lambda_{ex} = 362 \text{ nm}$) (inset are the solid state colors of 1Me before and after grinding).

Microscopic studies: 1H, when dissolved in THF shows bright cyan coloured fluorescence, atomic force microscopic (AFM) study with which $(1 \times 10^{-3} \text{ M})$ displays formation of mutually interconnected ring like structures of 800 nm dimension in average (Fig. S20, ESI†). Dynamic light scattering (DLS) study also suggests the same size distribution (Fig. S21, ESI†). Addition of up to 50% water in this increases the fluorescence intensity slightly (Fig. S22, ESI†), which could be due to the formation of fluorescent aggregates. Such aggregation is confirmed by the AFM analysis and DLS study. However, in acetonitrile, **1**H forms rectangular shaped microscopic crystal, which can easily be visible even under microscope, besides the AFM evidence.



Figure S24. AFM image of **1**H in THF, THF-water and acetonitrile showing interconnected ring-like structure formation in THF, aggregate formation in THF-water and rectangular crystal formation in acetonitrile; last one is the normal microscopic image.



Figure S25. DLS study of 1H in THF and 50% THF-water.



Figure S26. Change in PL intensity of THF solution of $1H (1 \times 10^{-5} \text{ M})$ in presence of increasing concentration of water; given are the % of THF.



Figure S27. Absorption titration spectra of 1H (10 μ M) with Al³⁺.



Figure S28. PL titration spectra of **1**H (10 μ M) with (a) Al³⁺ and (b) PPi.



Figure S29. Equivalent plot from PL titration data for 1H with (a) Al^{3+} and (b) PPi.

Calculation of detection limit. Detection limits (DL) were calculated using the following equation:

 $DL = (3 \times SD) / slope$

where, SD corresponds to the standard deviation of the blank sample, measured using 15 consecutive scans of the blank sample. The slope is obtained from the linear fit plot of PL intensity changes versus the concentration of guest added. The SD value of ligand **1**H was 702.24.



Figure S30. Calibration curve for (a) Al^{3+} and (b) PPi derived from corresponding PL titration data with **1**H (10 μ M) in acetonitrile at room temperature.



Figure S31. (a) Non-linear 1:1 fitting of PL titration data to calculate association constant of **1**H with Al³⁺ in acetonitrile at room temperature; (b) selectivity graph of **1**H with Al³⁺ in presence of other metal ions in acetonitrile (λ em= 435 nm for Al³⁺, Cr³⁺; 460 nm for other metal ions) as their perchlorate salt. Magenta bars represent the PL intensities of **1**H in presence of all metal ions (10 equiv) and blue bars correspond to the same in presence of all metal ions and Al³⁺. Codes used: (1) Only **1**H (2) Mg²⁺ (3) Fe³⁺ (4) Mn²⁺ (5) Cd²⁺ (6) Pb²⁺ (7) Zn²⁺ (8) Co²⁺ (9) Cu⁺ (10) Ni²⁺ (11) Ag⁺ (12) Hg²⁺ (13) Cr³⁺ (14) Al³⁺.

| Ref. | λ_{ex} (nm) | λ _{em} (nm) | Log K _a | LOD | Host-guest stoichiometry | Mode | Solvent |
|--|---------------------|-------------------------|-----------------------|------------|-----------------------------|-------------|---|
| ACS Sens., 2016, 1, 144 | 468 | 601 | 10.30 | 3.1 nM | 1:2 | Turn On | 10 μM in 0.1% DMSO/ HEPES |
| RSC Adv., 2014 , 4, 5845 | 317 | 441 | | 0.5 nM | 2:1 | Turn On | Water |
| J. Lumin., 2016, 172, 124 | 280 | 455 | 4.11 | 80 nM | 1:1 | Turn On | 5% DMSO-Water v/v, pH7 |
| Spectrochimica Acta Part A: Mol. Biomol. Spec., 2015 , 139, 119 | 450 | 506 | 4.10 | 0.99 μM | 1:1 | Turn On | CH ₃ CN-H ₂ O solution (1:1 v/v, HEPES 50 mM, pH = 7.0) |
| J. Phys. Chem. A, 2016 , 120, 210 | 364 | 426 | | 8.64 nM | 1:1 | Turn On | CH ₃ CN/H ₂ O, 95:5, v/v |
| <i>Tetrahedron Letters</i> , 2011 , 52, 5581 | 435 | 510 | 8.70 | 1.00 μM | 1:1 | Turn On | MeOH/aqueous HEPES buffer (1 mM, pH 7.4; 3:2 v/v) |
| Inorg. Chem., 2016 , 55, 9212 | 355 | 445 | 5.53 | 0.5 nM | 2:2 | Ratiometric | CH ₃ CN |
| | 366 | 463 | 4.90 | 12 nM | 1:1 | Ratiometric | 9:1 Water/CH ₃ CN, v/v |
| Present work | 365 | 435 | 4.54 | 7.62 nM | 2:2 | Ratiometric | CH ₃ CN |

| Tuble bar comparison of the sensing by the with some of the providesty reported sensors |
|---|
|---|

| Ref. | λ_{ex} | λ_{em} | Log | LOD | Host-guest | Mode | Solvent |
|--|----------------|----------------|--|-------------|--------------|-------------|--|
| | (1111) | (1111) | к _а | | storemometry | | |
| Org. Lett., 2008 , 10, 473-476 | 315 | 376 | 5.67 | | 2:1 | Turn Off | tris-HCl (0.01 M) solution (MeOH/H ₂ O) 1:9, v/v, pH 7.22 |
| <i>Org. Lett.</i> , 2011 , <i>13</i> , 1362-1365 | 430 | 512 | 4.10 | 2.18 μM | 2:1 | Turn On | HEPES buffer |
| <i>Tetrahedron Letters</i> , 2016 , <i>57</i> , 5022-5025 | 352 | 453 | 5.61 | | 1:1 | Turn Off | CH ₃ CN-HEPES buffer (0.02 M, pH 7.2) (v/v = 5:5) |
| New J. Chem., 2017 , 41, 4806-4813 | 350 | 450 | | 74 nM | 1:1 | Ratiometric | 6:4 (H ₂ O:EtOH, v/v) |
| <i>Inorg. Chem.</i> , 2016 , 55, 2212-2219 | 302 | 380 | 6.22 | 300 nM | 1:1 | Turn On | MOPS Buffer |
| Anal. Chem. 2013, 85, 8369-8375 | 350 | 480 | 4.24 | 2 ppb | 1:1 | Turn Off | MeOH/aqueous HEPES buffer (1 mM, pH 7.4; 3:2 v/v) |
| J. Am. Chem. Soc. 1999, 121, 9463-9464. | 312 | 476 | 8.08 ^a | | 2:1 | Turn On | МеОН |
| Inorg. Chem., 2009 , 48, 2993-2999 | 352 | 453 | 4.52 | | 1:1 | Turn On | 10 mM HEPES buffer solution (H_2O , pH 7.4) |
| Inorg. Chem. 2016, 55, 259-271. | 465 | 600 | 14.96 | 0.02 μM | 1:3 | Turn On | CH ₃ CN |
| J. Am. Chem. Soc., 2014, 136, 5543-5546 | 440 | 591 | | 0.8 nM | 3:1 | Turn On | 10 mM HEPES buffer (pH 7.4) |
| Dalton. Trans., 2018, 47 , 6819 (^a : K _{a1} ; ^b : K _{a2}) | 315 | 385 | 5.70 ^a , 5.26 ^b | 45.37 nM | 1:2 | Turn Off | 70% aqueous buffer (10 mM HEPES, pH 7.4) / acetonitrile |
| Present work | 365 | 478 | | 5.67 nM | 2:1 | Ratiometric | CH ₃ CN |

 Table S3. Comparison of PPi sensing by 1H with some of the previously reported sensors.



Figure S32. ESI-MS spectra of the Al^{3+} adduct of **1**H and the isotopic distribution pattern of $[Al(1)O]_2K^+$ with its corresponding simulated pattern.



Figure S33. Isotopic distribution pattern of $[(1H)_2 + H_2P_2O_7^{2-} + 3Na^+]^+$ with the corresponding simulated pattern.



Figure S34. Emission spectral change of 1Me in presence of Al³⁺.

References:

- SAINT and XPREP, 5.1 ed.; Sheldrick, G. M., Ed.; Siemens Industrial Automation Inc: Madison, WI, 1995.
- SADABS, Empirical Absorption Correction Program; University of Göttingen: Germany, 1997.
- 3. Sheldrick, G. M. SHELXTL Reference Manual, Version 5.1; Bruker AXS: Madison, WI, 1997.
- 4. Sheldrick, G. M. SHELXL-97, Program for Crystal Structure Refinement; University of Göttingen: Germany, 1997.
- 5. Spek, A. L. PLATON-97; University of Utrecht: The Netherlands, 1997.
- 6. Mercury 3.1 (supplied with Cambridge Structural Database); CCDC, Cambridge, U.K, 2004.
- 7. G. S. Kumar, R. Roy, D. Sen, U. K. Ghorai, R. Thapa, N. Mazumder, S. Saha, and K. K. Chattopadhyay, *Nanoscale*, 2014, **6**, 3384.
- (a) C.-C. Hsieh, C.-M. Jiang, P.-T. Chou , *Acc. Chem. Res.* 2010, **43**, 1364; (b) Y. Peng, Y. Ye, X. Xiu and S. Sun, *J. Phys. Chem. A*, 2017, **121**, 5625; (c) J. Seo, S. Kim, S. Y. Park, *J. Am. Chem. Soc.*, 2004, **126**, 11154; (d) L. Chen, D. Wu and J. Yoon, *Sens. and Actuators B*, 2018, **259**, 347;