CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

A Fluorescent Switch-based Computing Platform in Defending Information Risk

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Supporting Information for

A Fluorescent Switch-based Computing Platform in Defending Information Risk

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I. Photophysical properties of MPTEA and its derivatives.

II. Additional notes for authentication process.

III. Additional schemes for the operations of secured molecular platform.

I. Photophysical properties of MPTEA and its derivatives.

All the spectral characterizations were carried out in acetonitrile (HPLC grade) solution at room temperature with a 10 mm quartz cell. The concentration is listed in the footnote of each figure. The UV-vis absorption spectra were measured with a Shimadzu UV-3100 spectrometer, and the fluorescence emission spectra were recorded upon the excitation at 350 nm on a Hitachi F-4500 fluorescence spectrometer. The quantum yield was measured at room temperature with the excitation at 350 nm (Xe lamp in the F-4500 spectrometer). Quinine sulfate dihydrate in dilute sulfuric acid solution (Φ_{fr} = 0.546) is selected as the reference. The calculation of quantum yield is according to the equation 1.[1]

$$\Phi = \Phi_{fr} \times \frac{1-10^{-ArLr}}{1-10^{-AL}} \times \frac{N^2}{N_r^2} \times \frac{D}{D_r} \qquad \text{(Equation 1)}$$

(1) J. N. Demas, G. A. Grosby, *J. Phys. Chem.* **1971**, *75*, 991–1024.

Table S1. Photophysical properties of MPTEA, Ad, and H_2M in acetonitrile.

	λ_{abs} / nm	log (ε_{max} / $mol^{-1}\cdot L\cdot cm^{-1}$)	λ_{em} / nm	Φ	τ / ns
MPTEA	355, 307	4.2, 4.6	525	0.025	1.25
Ad	355, 307	4.2, 4.5	435	0.028	2.89
H_2M	400, 300	4.3, 4.2	500	0.194	0.29

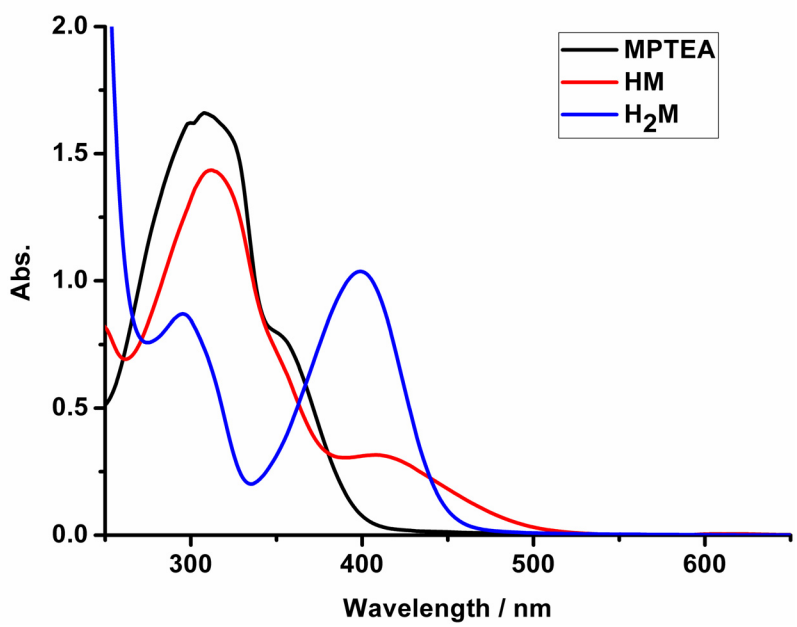


Figure S1. The absorption spectra of MPTEA (black line), HM (red line) and H_2M (blue line) in acetonitrile solution (concentration of each compound is 0.02 mmol·L^{-1}).

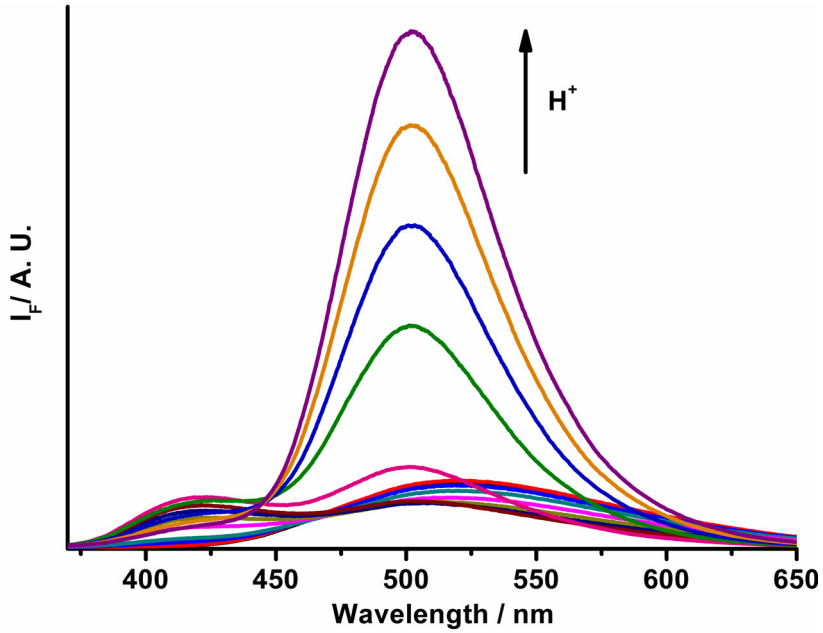


Figure S2. Fluorescent spectra of MPTEA (0.02 mM) in acetonitrile solution upon addition of different concentration trifluoroacetic acid (from 0, 1×10^{-4}, 1×10^{-3}, 2×10^{-3}, 4×10^{-3}, 6×10^{-3}, 8×10^{-3}, 1×10^{-2}, 2×10^{-2}, 4×10^{-2}, 6×10^{-2}, and 8×10^{-2} to 0.1 mol·L^{-1}).

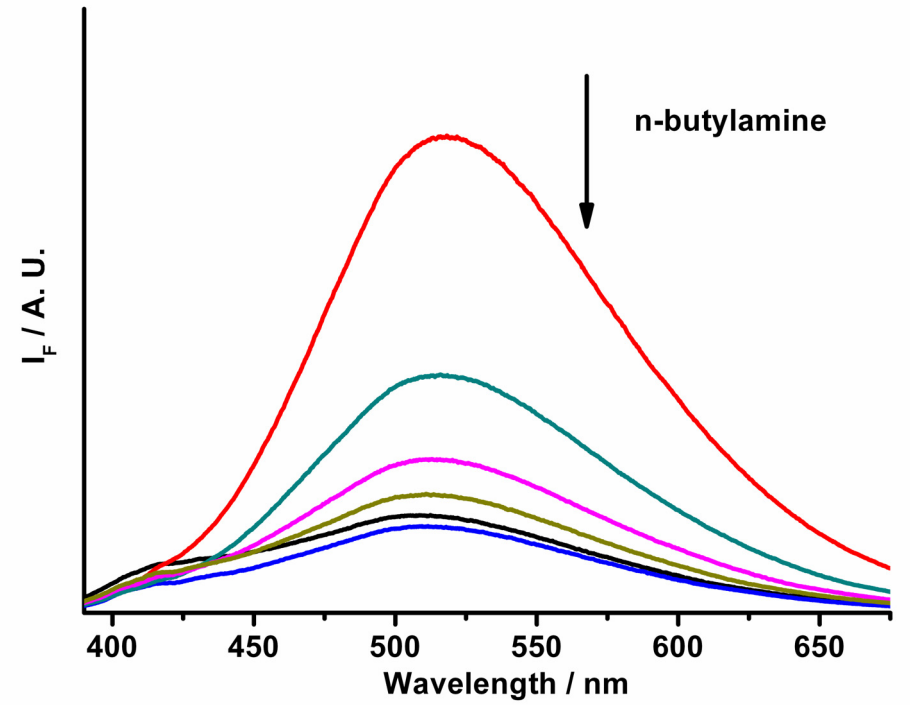


Figure S3. Fluorescent spectra of MPTEA (0.02 mmol·L^{-1}) in acetonitrile solution upon addition of different concentrations of *n*-butylamine.

II. Additional notes for authentication and encryption processes.

Table S2. MPTEA binding forms of the 16 selected possibilities in Figure 2b.

Number string	1111	1121	1131	1141	1211	1221	1231	1241
MPTEA form	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA
Number string	1311	1321	1331	1341	1411	1421	1431	1441
MPTEA form	MPTEA	MPTEA	H_2M	Cu-Ad	MPTEA	MPTEA	MPTEA-Cu	MPTEA

.

Table S3. MPTEA binding forms of the 27 selected possibilities in Figure 2c.

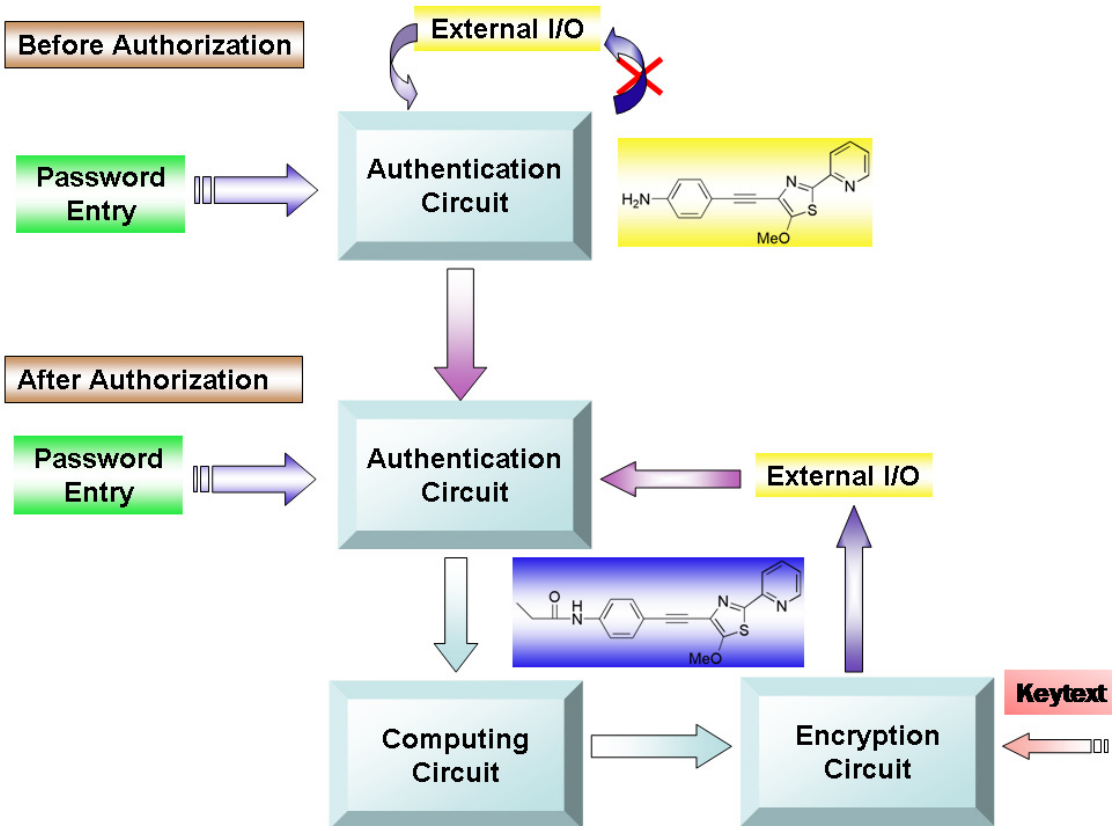
Number String	2221	2231	2241	2321	2331	2341	2421	2431	2441
MPTEA form	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA	MPTEA
Number String	3221	3231	3241	3321	3331	3341	3421	3431	3441
MPTEA form	MPTEA	MPTEA	MPTEA	MPTEA	H_2M	MPTEA-Cu	Ad	Ad-Cu	Ad-Cu
Number String	4221	4231	4241	4321	4331	4341	4421	4431	4441
MPTEA form	MPTEA	MPTEA	MPTEA	MPTEA	Ad-Cu	Ad-Cu	MPTEA	MPTEA-Cu	MPTEA

Introduction of different keytexts can tune protonation forms of MPTEA binding states, which produce optical ciphertext. The binding forms of encryption processes in Table 1 are listed as follows. Based on the acidobasic properties of keytexts, the encrypted arithmetic results can be decrypted.

Table S4. Binding forms of plaintexts and ciphertexts in Table 1.

Operation	Binding Forms for Original Output	Keytext	Encrypted Output	Binding Forms for Encrypted Output
00-10-01-00-10-01	Ad, Ad-Cu, HAd, Ad, Ad-Cu, HAd.	ANBANN	10-10-10-10-10-01	Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, HAd.
10-10-01-00-10-01	Ad-Cu, Ad-Cu, HAd, Ad, Ad-Cu, HAd.	NNBANN	10-10-10-10-10-01	Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, HAd.
10-01-01-00-10-01	Ad-Cu, Ad-Cu, HAd, Ad, Ad-Cu, HAd.	NBBANN	10-10-10-10-10-01	Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, HAd.
10-01-00-00-10-01	Ad-Cu, Ad-Cu, Ad, Ad, Ad-Cu, HAd.	NBAANN	10-10-10-10-10-01	Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, Ad-Cu, HAd.

III. Additional scheme for the operations of secured molecular platform.



Scheme S1. Illustration of the molecular secured platform converting from the unauthorized stand-by state to the authorized user 2's operation state.