Supporting Information

Pb^{2+} Induced DNA Conformational Switch from Hairpin to G-quadruplex: Electrochemical Detection of Pb^{2+}

Zhenzhen Lin,[†] Yue Chen,[†] Xiaohong Li,[†]* Weihai Fang[†]*
Department of Chemistry, Beijing Normal University, Beijing, 100875, China

Experimental

DNA sequences and preparation of Monolayer Preparation (The underlined are complementary pairs).

DNA(1): 5′-HO-$(CH_2)_6$-SS-$(CH_2)_6$-TTTTT-CCAAC-GGTTGG-TGT-GGTTGG-3′

DNA(2): 5′-TTTTT-CCAAC-GGTTGG-TGT-GGTTGG-3′

DNA(3): 5′-HO-(CH2)6-SS-(CH2)6-CGT-GCG-GAT-TTT-CCA-CTT-GCT-GTG-CGC-ACG-3′

Newborn Calf serum were purchased from invitrogen corportion(New Zealand) and diluted with 20 mM Tris-ClO_4 buffer ten times for use.

Films of hairpin DNA (1) and DNA (3) were prepared by incubating freshly cleaned gold electrodes in solutions of 10 μM DNA strand (1), followed by soaking the film in 1 mM 6-mercaptohexanol in 20 mM Tris-ClO_4. The EIS of the films were recorded.

Theoretical Computation. The hairpin DNA chain has 20 nuclei acid units. All the phosphate moieties were replaced by phosphate ester. Then the whole molecule has 726 atoms. Density functional CAM-B3LYP[1] implemented in Gaussian 09 program package[2] were employed to optimization the structures with mixed basis sets, where 3-21G* was used for C, N, O and H atoms and 6-31G* for P atoms and LANL2DZ for Pb atom.

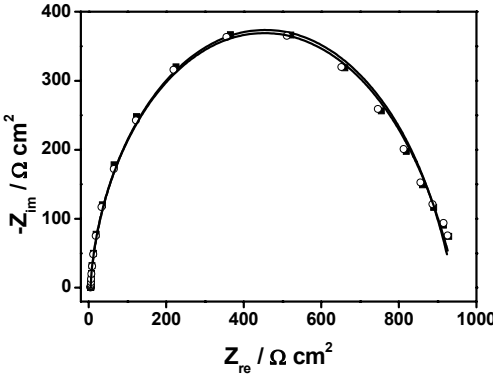

Figure S1. Representative Nyquist plots ($-Z_{im}$ vs Z_{re}) for films of hairpin DNA (3) before(■) and after incubating with 50 μM $PbClO_4$ solution after t buffer washing(○).

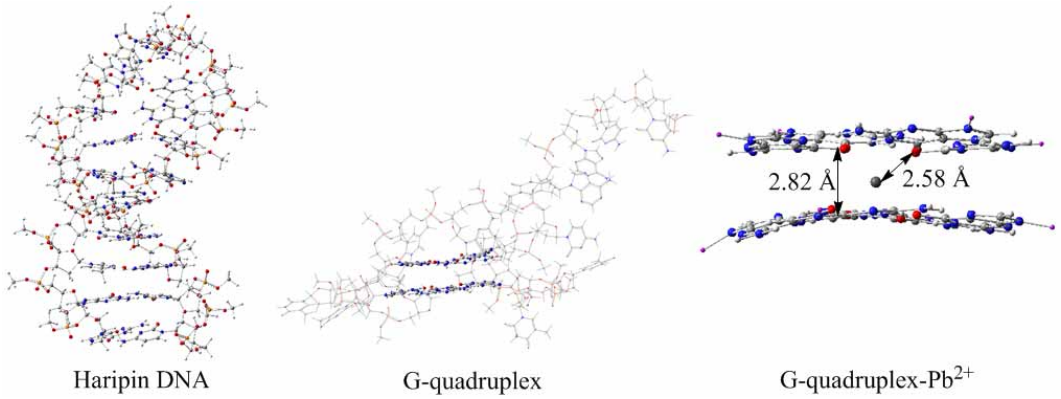

Figure S2. The optimized structures of hairpin DNA, G-quadruplex (without Pb^{2+}) and G-quadruplex-Pb^{2+}. For clarity, some parts of G-quadruplex-Pb^{2+} were hidden.

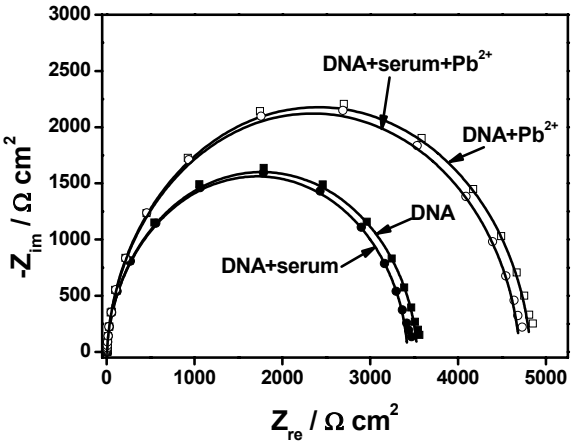

Figure S3. Representative Nyquist plots ($-Z_{im}$ vs Z_{re}) for films of hairpin DNA (1) (■) ;DNA (1) incubated in serum(●); DNA (1) incubated in 50 μM $PbClO_4$ solution(□); DNA (1) incubated in the mixture of serum and 50 μM $PbClO_4$ solution(○).

Table S1. Summary of the assays for Pb^{2+} detection reported by other authors [a]

Methods	DNA Sequence	Transduer	Detection Range	Detection Limit
DNAzyme sensor based on electrode-bound DNAzyme assembly[3]	8-17 DNAzyme	electrochemical	0.5μM - 10μM	0.3μM
DNA-Au Bio-Bar codes[4]	8-17 DNAzyme	electrochemical	5nM - 0.1μM	1 nM
DNAzyme sensor based on functionalized gold nanoparticles[5]	8-17 DNAzyme	electrochemical	0.1nM - 35nM	28pM
DNAzyme sensor based on catalytic and molecular beacon[6]	8-17 DNAzyme	fluorescent	3nM - 5μM	0.6 nM
DNAzyme sensor based on abasic site-containing DNAzyme[7]	8-17 DNAzyme	fluorescent	0 - 1μM	4 nM
DNAzyme sensor based on GR-5 DNAzyme[8]	GR-5 DNAzyme	fluorescent	25nM - 2μM	3.7nM
Sensor based on thrombin-binding aptamer with 5′-FAM and 3′-DABCYL[9]	thrombin-binding aptamer	fluorescent	0.5nM - 30nM	0.3nM
Label-free colorimetric cetection based on gold nanoparticles and DNAzyme[10]	8-17 DNAzyme	colorimetric	3nM - 100nM	3 nM
DNAzyme cascades[11]	8-17 DNAzyme	colorimetric or chemiluminescence	10 nM -10μM	10 nM
Sensor based on Lead(II)-Induced Allosteric G-Quadruplex DNAzyme[12]	G-quadruplex DNAzyme PS2.M	colorimetric or chemiluminescence	0.1 μM-10 μM or 1nM-$10^{-6.5}$M	32nM/ 1nM

a The bibliographic reference, methods, DNA sequence, transduer, detection range and detection limit reported by authors are reviewed.

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