Supporting Information for

Selective Decomposition of Aqueous Nitrate into Nitrogen using Iron Deposited Bimetals

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The supporting information consists of 3 pages, including 2 figures.

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Reagent. Potassium nitrate and sodium nitrite were purchased from Aldrich (99+%, Milwaukee, WI). The buffer, N-[2-hydroxyethyl]piperazine-N'- [2-ethanesulfonic acid] acid (HEPES, Sigma), was added to control the pH of the solution between 5.5 to 8.5, and resulting in a pH change less than 0.3. The zerovalent iron used was iron powder (99.6%, finer than 100 mesh) obtained from J. T. Baker. Copper(II) chloride were supplied by Alfa. The catalytic bimetallic precursors, including K₂PdCl₆, K₂PtCl₆, and HAuCl₄ • 4H₂O, were supplied by Aldrich. All aqueous solutions were made in water purified with a Milli-Q system (18.2 M Ω /cm). The desired concentrations of nitrate, 40 mg-N/L, in Ar-purged water were prepared by dilution of a 1000 mg-N/L stock solution.

Oxidation number	Formula	Remarks	Physical-chemical methods
+5	NO ₃ ⁻	Substrate	
+4	NO_2	No information	_*
+3	NO ₂ ⁻	Known intermediate	Hydrogenation with catalysts (5); photocatalytic (8); zerovalent iron (17, 20, 23, 26, 27); zerovalent zinc (34)
+2	NO	Hypothetical intermediate	Hydrogenation with catalysts (5)
+1	N_2O	Known intermediate	Hydrogenation with catalysts (6)
0	N ₂	Known product	Hydrogenation with catalysts (5, 6); photocatalytic (7, 8); nanoscale zerovalent iron (26, 29, 30); zerovalent aluminum (35)
-1	NH ₂ OH	No information	_*
-2	N_2H_4	No information	_*
-3	NH ₃ /NH ₄ ⁺	Known product	Hydrogenation with catalysts (5); photocatalytic (8); zerovalent iron at neutral pH (17, 20, 23, 26, 27); zerovalent zinc (34); zerovalent Al (35);nanoscale zerovalent iron (26,29,3)

Table S1 Possible nitrogen compounds involved in aqueous nitrate reduction using physical-chemical methods.

*No data found in the literature.

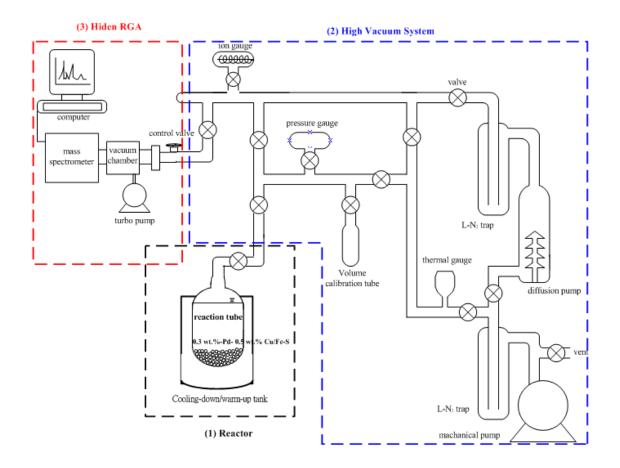


Figure S1. The apparatus of gas analysis system consisting of three parts including reactor, high-vacuum system and Hiden RGA. The mixture of isopropanol and liquid nitrogen at the temperature of -40 °C - 50 °C was used to rapidly convert aqueous solution into solid phase, and then the air was extracted by the high-vacuum system (< 10^{-5} torr). After switching off the valve, a heat gun was used to warm up the solution to room temperature. For certain reaction period, the solution was cooled down again. Switching on the valve for measuring the total pressure of the produced gas by the pressure gauge. The dead volume of the system calibrated by a volume tube is 80 cm³. The produced gas was then introduced into the Hiden RGA through a needle valve. The routine QA measures of accuracy and precision have well done for the gas analysis system. The recovery of the standard N₂ gas is 95%-102%; the standard deviation (σ) is 0.0002 mg-N for N₂ gas, and the instrument detection limit (IDL=3 σ) is 0.0006 mg-N.

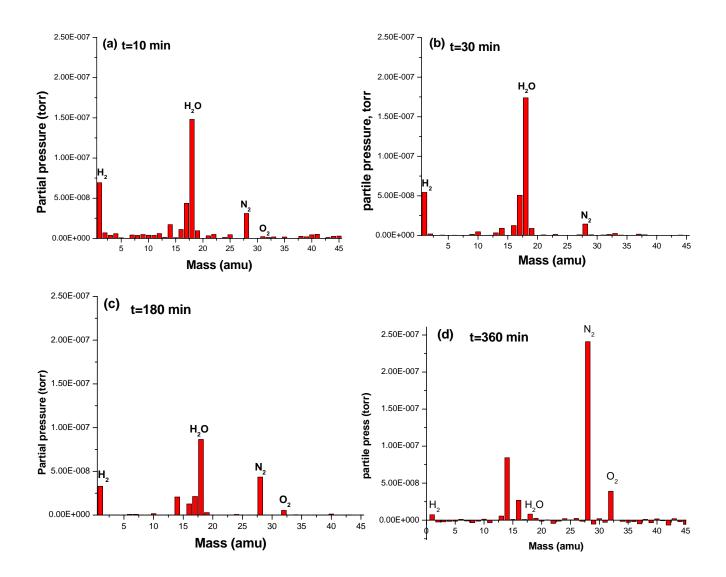


Figure S2. RGA partial pressure measurement in the mass-range of 1-46 amu for the reaction of 40 mg-N/L nitrate by 0.5 g 0.3 Pd- 0.5 Cu/Fe-S.

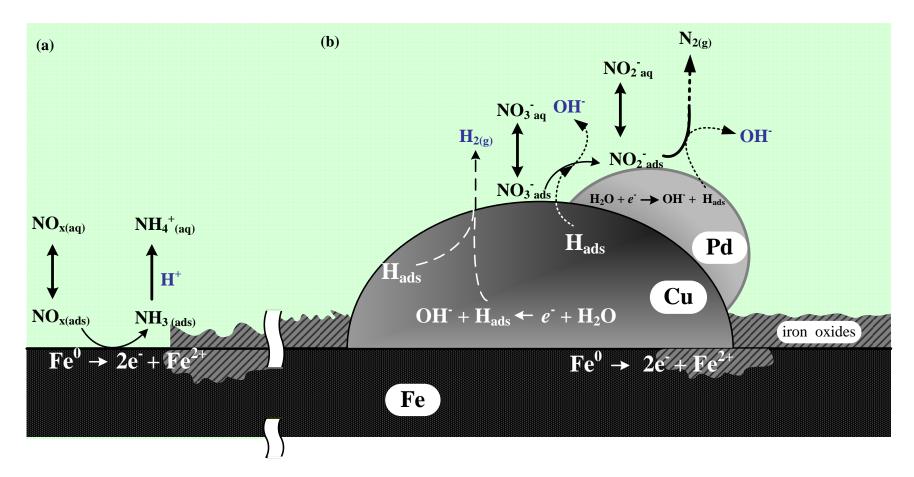


Fig S3 Aqueous nitrate removal via: (a) directly reduction by electron; (b) abstraction of oxygen by H_{ads}.