

Electronic Supplementary Information

Mapping the Reactions of Hexavalent Chromium [Cr(VI)] in Iron
Nanoparticles with Aberration Corrected Scanning Transmission
Electron Microscopy (Cs-STEM)

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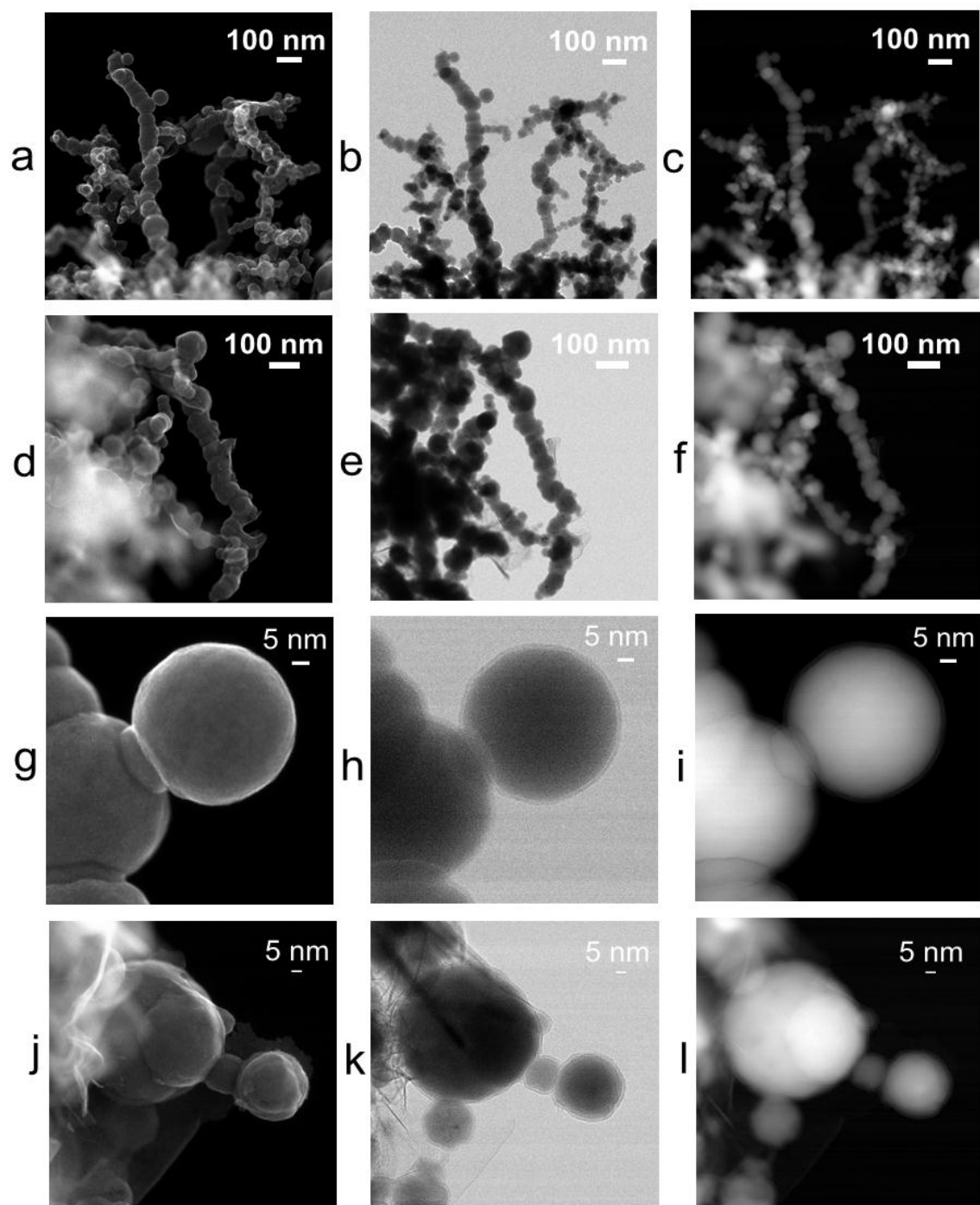


Figure S1. STEM images of nanoscale zero-valent iron (nZVI): (a) to (c) and (g) to (i) are fresh nZVI, (d) to (f) and (j) to (l) are after 24 h reactions with 100 mg L^{-1} Cr(VI). (a), (d), (g), and (j) are SE images, (b), (e), (h) and (k) BF images, (c), (f), (i) and (l) HAADF images.

Low-resolution images of nZVI illustrate the degree of aggregation and particle-particle interactions before (Figure S1a-S1c) and after (Figure S1d-S1f) reactions with $100 \text{ mg L}^{-1} \text{ Cr(VI)}$.

After reactions with Cr(VI), the spherical shape of nZVI is distorted due to surface oxidation and iron hydroxide precipitation, with irregular grain boundaries and bumpy surfaces, and with newly formed deposits on the surface (Figure S1j-S1l). As shown in the above figure, the individual particles were slightly smaller, but sizes of the particle aggregates were significantly larger with progressive aggregation. Nonetheless, individual particles still preserve the core-shell structure but with increased shell thickness.

In Figure S1d-S1f, the images of spent nZVI clusters after reaction with dichromate show that loosely aggregated materials, likely from precipitates from the solution on the nZVI surface. Significant changes are also observed at the particle-particle interactions with much larger (e.g., microscale) aggregates glued together by the iron hydroxides from iron oxidation.

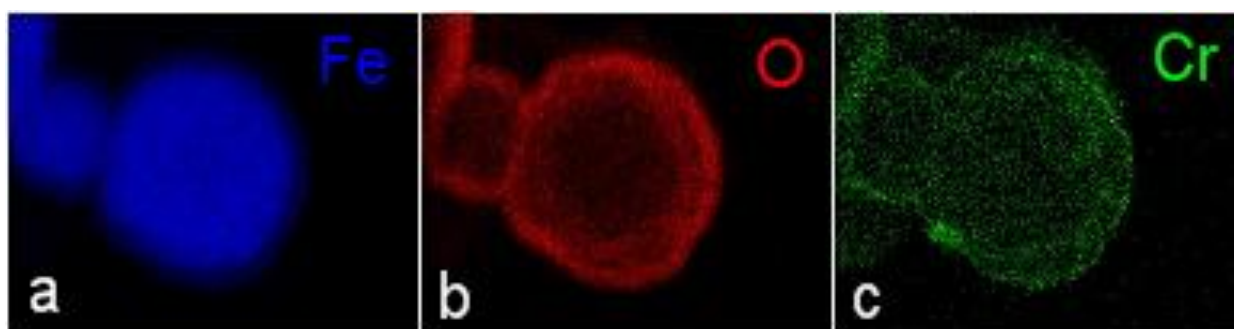


Figure S2. STEM-XEDS elemental mapping of Fe(a), O(b), Cr(c) emphasize the spatial extent of each signal over a whole nZVI particle. Signals collected from nZVI reacted with 100 mg L^{-1} dichromate.

Methods for chromium analysis. At the pre-determined reaction time, aqueous samples were filtered through filter paper (Whatman, #2) for measurements of dissolved Cr concentration. Total dissolved chromium was determined by the method of ICP-OES. An ICP-Agilent720ES was used, which has a detection limit of 1~4 ppb.