

# Electrically conductive magnetic nanowires using an electrochemical DNA-templating route.

*Scott M. D. Watson,<sup>a</sup> Hasan Daw A. Mohamed,<sup>a,b</sup> Benjamin R. Horrocks,<sup>a</sup> Andrew Houlton\*<sup>a</sup>*

<sup>a</sup>Chemical Nanoscience Laboratory, School of Chemistry, Newcastle University,  
Newcastle-Upon-Tyne, NE1 7RU (UK)

<sup>b</sup>Chemistry Department, Faculty of Arts and Science, Azzaytuna University,  
P.O. Box 39011/39010, Tarhuna, Libya

**Supporting Information**

### FT-IR spectroscopy

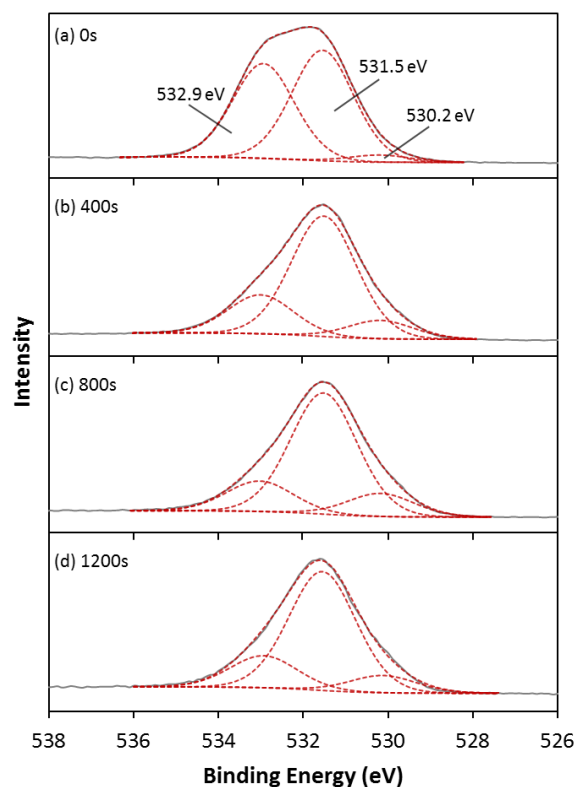
**Table S1.** Assignment and comparison of FTIR spectra (400–4000 $\text{cm}^{-1}$ ) of calf thymus DNA, and calf thymus DNA following association of with  $\text{Fe}^{2+}$  cations in aqueous solution.

| Wavenumber ( $\text{cm}^{-1}$ ) |                           | Assignment <sup>a</sup>   |
|---------------------------------|---------------------------|---|
| CT-DNA                          | CT-DNA / $\text{Fe}^{2+}$ |   |
| 961                             | 973                       | C-C deoxyribose stretch   |
| 1021 <sup>b</sup>               | -                         | C-O deoxyribose stretch   |
| 1071                            | 1066                      | P-O/C-O deoxyribose stretch   |
| 1097                            | 1103                      | $\text{PO}_2^-$ symmetric stretch                                       |
| 1244                            | 1205                      | $\text{PO}_2^-$ asymmetric stretch                                      |
| 1364                            | 1368                      | C-N stretch of cytosine / guanine                                       |
| 1417                            | 1419                      | C-H / N-H deformation; C-N stretch                                      |
| 1487                            | 1487                      | Ring vibration of cytosine / guanine                                    |
| 1530                            | 1531                      | In-plane vibration of guanine / cytosine                                |
| 1605                            | 1602 <sup>b</sup>         | In-plane vibration of adenine   |
| 1652                            | 1654                      | C=O stretch of cytosine / thymine (?);<br>In-plane vibration of thymine |
| 1688                            | 1681                      | C=O stretch of guanine / thymine;<br>N-H thymine                        |
| 2850–3500                       | 2850–3500                 | C-H / N-H / O-H stretches   |

<sup>a</sup> Assignments of DNA vibration bands reference to [1–4].

<sup>b</sup>Peak appeared as a shoulder.

### X-ray photoelectron spectroscopy

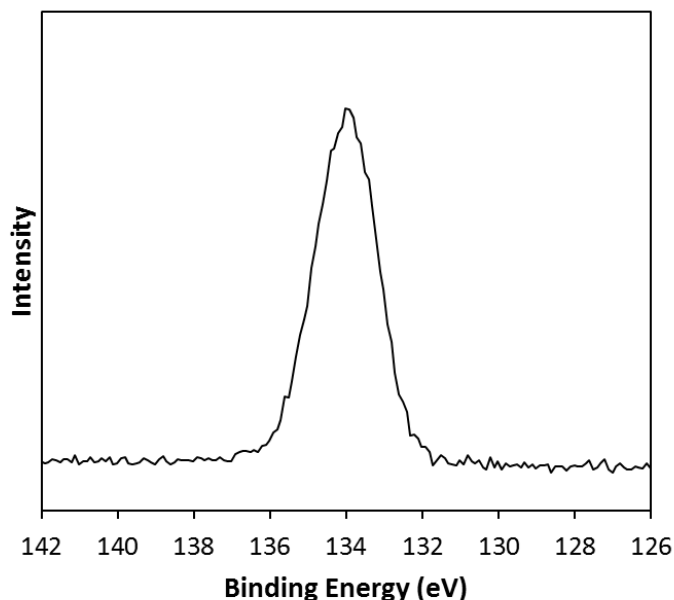


**Figure S1.** Curve-fitting of high resolution XP spectra of the O1s region from DNA-templated Fe nanowires, prepared via electrochemical reduction of  $\text{Fe}^{2+}$  in the presence of DNA. The spectra were acquired following etching of the nanowires by  $\text{Ar}^+$  sputtering for a period of (a) 0s, (b) 400s, (c) 800s, and (d) 1200s.

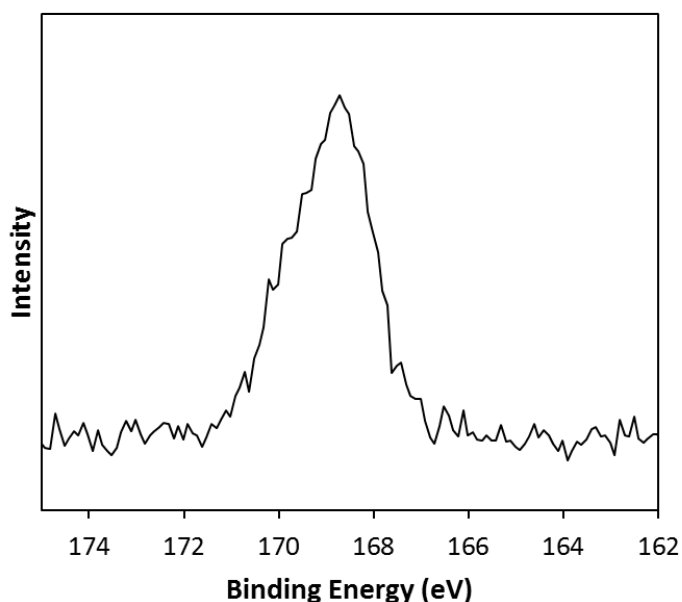
From XPS depth profile studies of the DNA-templated Fe material, analysis of the Fe2p spectra determined the electrodeposited Fe to possess a core-shell structure comprised of a metallic Fe nucleus encased by a surface oxide layer, deduced to be oxide (*e.g.*  $\text{Fe}_2\text{O}_3$ ,  $\text{Fe}_3\text{O}_4$ ) or oxyhydroxide ( $\text{FeOOH}$ ) (see main manuscript for details). This was supported by curve-fitting of the O1s spectra.

As numerous different oxygen types are present in the product material (*e.g.* oxygen present in iron oxide/hydroxide, DNA,  $\text{FeSO}_4$ ), making accurate fitting of the O1s spectra non-trivial, a simplified approach has been taken here. A minimum of three components are required in order to accurately reproduce the shape of the O1s spectra, where each component is the sum of several contributions, see Figure S1. The component at highest binding energy (532.9eV) is attributed to oxygen atoms in the DNA phosphate groups<sup>5, 6</sup> (Note: the presence of a P2p signal around 134.1eV (see Figure S2) is consistent with this). Other contributions to this component of the O1s envelope are expected from the sulfate groups of unreacted  $\text{FeSO}_4$  starting material present in the sample<sup>7, 8</sup> (the presence of the sulfate groups is also indicated from the S2p signal observed around 168.7 eV, see Figure S3), as well as  $\text{H}_2\text{O}$  adsorbed at the surface of the Fe structures.<sup>9, 10</sup> The second component in the O1s envelope (531.5eV), of similar intensity to the first, can be assigned to oxygen atoms present in the sugar and nucleobase units of the DNA.<sup>5, 6</sup> A contribution from the underlying  $\text{SiO}_2$  substrate to the

spectrum within the region of these first two components may also be present, though this is not expected to be significant due to the considerable amount of sample material present on top of the substrate (this is supported by the XPS survey scan which showed only a weak Si2p signal). The final component fitted within the O1s envelope (530.2eV) is in reasonable agreement with the expected binding energy for O<sup>2-</sup> species found in iron oxides.<sup>7,9,10</sup> This is consistent with the Fe nanostructures possessing an oxide layer at their surface.



**Figure S2.** High resolution XP spectra of P2p region acquired from a sample of DNA-templated Fe nanowires.



**Figure S3.** High resolution XP spectra of S2p region acquired from a sample of DNA-templated Fe nanowires.

## References

- [1] S. Alex and P. Dupuis, *Inorganica Chimica Acta*, 1989, **157**, 271-281.
- [2] A.A. Ouameur and H.-A. Tajmir-Riahi, *J. Biol. Chem.*, 2004, **279**, 42041-42054.
- [3] H. Arakawat, R. Ahmad, M. Naoui and H.-A. Tajmir-Riahi, *J. Biol. Chem.*, 2000, **275**, 10150-10153.
- [4] G.I. Dovbeshko, N.Y. Gridina, E.B. Kruglova and O.P. Pashchuk, *Talanta*, 2000, **53**, 233-246.
- [5] C.-Y. Lee, P. Gong, G.M. Harbers, D.W. Grainger, D.G. Castner, and L.J. Gamble, *Anal. Chem.*, 2006, **78**, 3316-3325.
- [6] M.R. Vilar, A.M. Botelho do Rego, A.M. Ferraria, Y. Jugnet, C. Noguès, D. Peled, and R. Naaman, *J. Phys. Chem. B*, 2008, **112**, 6957-6964.
- [7] A.P. Grosvenor, B.A. Kobe, M.C. Biesinger, and N.S. McIntyre, *Surf. Interface Anal.*, 2004, **36**, 1564-1574.
- [8] B.J. Lindberg, K. Hamrin, G. Johansson, U. Gelius, A. Fahlman, C. Nordling, and K. Siegbahn, *Phys. Scripta*, **1970**, 1, 286-298.
- [9] X.-Q. Li, and W.-X. Zhang, *J. Phys. Chem. C*, **2007**, 111, 6939-6946.
- [10] X.-Q. Li, and W.-X. Zhang, *Langmuir*, **2006**, 22, 4638-4642.