Supplementary materials

Design of optimally stable molecular coatings for Fe-based nanoparticles in aqueous environments

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1 surface terminations

In Figures S1 to S12 we have plotted the cementite and magnetite surfaces (001), (010), (100), (110), and (111). Figures S1 to S5 correspond to cementite surfaces, while Figures S6 to S12 correspond to magnetite surfaces. The figures show, in green arrows and numbers, the distance between the Fe atoms, which are the adsorption sites. Some atoms are labeled with “SL” marks. These are atoms located in the second layer and therefore are not adsorption sites. It is important to mention that in the case of magnetite (110) there are two possible terminations (see Figures S7 and S8). While for the case of magnetite (111) we have four possible terminations (see Figures S9, S10, S11, and S12).

The figures show that the distance between Fe atoms, in cementite surfaces, range from 2.4 to 3.9 Å. This allows for the bidentate and tridentate binding of the molecules. On the other hand, the figures show that the distance between Fe atoms, in magnetite surfaces, are larger than the ones in cementite, ranging from 2.9 to 5.9 Å. Therefore, not in all surfaces the molecules are able to bind in tridentate fashion. Furthermore, on the magnetite (111) surface, termination #4 (see Figure S12), the distance between atoms is so large (5.9 Å), that the molecules under consideration are only able to bind in a monodentate fashion.
Figure S1: Cementite (001) surface. Green labels denote the distance between Fe atoms (adsorption sites).
Figure S2: Cementite (010) surface. Green labels denote the distance between Fe atoms (adsorption sites).
Figure S3: Cementite (100) surface. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.

Figure S4: Cementite (110) surface. Green labels denote the distance between Fe atoms (adsorption sites).
Figure S5: Cementite (111) surface. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.
Figure S6: Magnetite (001) surface. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites. The other two surfaces, (010) and (100), are identical to the (001) surface shown in this figure.
Figure S7: Magnetite (110) surface termination #1. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.
Figure S8: Magnetite (110) surface termination #2. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.
Figure S9: Magnetite (111) surface termination #1. Green labels denote the distance between Fe atoms (adsorption sites).

Figure S10: Magnetite (111) surface termination #2. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.
Figure S11: Magnetite (111) surface termination #3. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.

Figure S12: Magnetite (111) surface termination #4. Green labels denote the distance between Fe atoms (adsorption sites). The atoms labeled with “SL” are atoms located in the second layer, and are not adsorption sites.