Supplementary Materials

A theoretical investigation on sulfidated nanoscale zero valent iron for removal of cis-DCE and PCE

Jessica Jein White[1], Ming Zhou[1], Jack Jon Hinsch[1], William W. Bennett[2], Yun Wang[1]

[1]Centre for Catalysis and Clean Energy, School of Environment and Science, Griffith University, Gold Coast Campus, Southport, Queensland 4222, Australia.

[2]Coastal and Marine Research Centre, Cities Research Institute, Griffith University, Gold Coast Campus, Queensland 4222, Australia.

Correspondence to: Prof. Yun Wang, Centre for Catalysis and Clean Energy, School of Environment and Science, Griffith University, Gold Coast Campus, 1 Parklands Drive, Southport, Queensland 4222, Australia. E-mail: yun.wang@griffith.edu.au

Table S1: Distance between listed atoms for molecular adsorption of cis-DCE on Fe(110).

Cis-DCE 110	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73

Table S2: Distance between listed atoms for molecular adsorption of cis-DCE on Fe(211).

Cis-DCE 211	Distance (Å)
C-C	1.46
C-H	1.10
C-H	1.09
C-Cl	1.92
C-Cl	1.82

Table S3. Distance between listed atoms for molecular adsorption of cis-DCE on HC-Fe(110).

Cis-DCE HC 110	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73

Table S4. Distance between listed atoms for molecular adsorption of cis-DCE on HC-Fe(211).

Cis-DCE HC 211	Distance (Å)
C-C	1.33
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73

Table S5. Distance between listed atoms for molecular adsorption of PCE on HC-Fe(110).

PCE HC 110	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72

Table S6. Distance between listed atoms for molecular adsorption of PCE on HC-Fe(211).

PCE HC 211	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72

Table S7. Distance between listed atoms for molecular adsorption of cis-DCE on LC-Fe(110).

Cis-DCE Low Coverage 110 (1)	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73
Cl-S	3.56

Table S8. Distance between listed atoms for molecular adsorption of cis-DCE on LC-Fe(110).

Cis-DCE Low Coverage 110 (2)	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73
Cl-S	3.47
Cl-S	3.61

Table S9. Distance between listed atoms for molecular adsorption of cis-DCE on LC-Fe(211).

Cis-DCE Low Coverage 211 (1)	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.08
C-Cl	1.73
C-Cl	1.73
Cl-S	3.74

Table S10. Distance between listed atoms for molecular adsorption of cis-DCE on LC-Fe(211).

Cis-DCE Low Coverage 211 (2)	Distance (Å)
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73
Cl-S	3.74
Cl-S	3.93

Table S11. Distance between listed atoms for molecular adsorption of PCE on Fe(110).

PCE 110	Distance (Å)
C-C	1.36
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72

Table S12. Distance between listed atoms for molecular adsorption of PCE on Fe(211).

PCE 211	Distance (Å)
C-C	1.36
C-Cl	1.72
C-Cl	1.72
C-Cl	1.73
C-Cl	1.72

Table S13. Distance between listed atoms for molecular adsorption of PCE on LC-Fe(110).

PCE Low Coverage 110 (1)	Distance (Å)
C-C	1.36
C-Cl	1.72
C-Cl	1.71
C-Cl	1.72
C-Cl	1.72
Cl-S	3.56
Cl-S	3.52
Cl-S	3.60
Cl-S	3.50

Table S14. Distance between listed atoms for molecular adsorption of PCE on LC-Fe(110).

PCE Low Coverage 110 (2)	Distance (Å)
C-C	1.36
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
Cl-S	3.45

Table S15. Distance between listed atoms for molecular adsorption of PCE on LC-Fe(211).

PCE Low Coverage 211 (1)	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.73
Cl-S	3.60

Table S16. Distance between listed atoms for molecular adsorption of PCE on LC-Fe(211).

PCE Low Coverage 211 (2)	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
Cl-S	3.86
Cl-S	3.77

Table S17. Charge Transfer Analysis of cis-DCE and PCE on Fe Surfaces.

Surface	Bader Charge – PCE (e^-)	Bader Charge – cis-DCE (e^-)
110	0.02	0.08
110LC	0.13	0.12
110LC	0.07	0.13
110HC	0.05	0.02
211	0.14	0.50
211LC	0.03	0.12
211LC	0.09	0.23
211HC	0.00	0.04

Table S18. Distance between listed atoms for dissociative adsorption of PCE on Fe(211).

211 PCE	**Distance (Å)**
Fe-Cl	2.33, 2.34
Fe-Cl	2.29, 2.35
Fe-Cl	2.32, 2.34, 3.64
C-Cl	1.72
C-Fe	1.84, 1.77
C-Fe	1.92, 1.80, 1.99, 1.80

Table S19. Distance between listed atoms for dissociative adsorption of cis-DCE on Fe(211).

211 cis-DCE	**Distance (Å)**
Fe-Cl	2.32, 2.35
Fe-Cl	2.41, 2.29
C-C	1.33
C-H	1.10, 1.09

Table S20. Distance between listed atoms for dissociative adsorption of PCE on LC-Fe(211).

211 LC PCE	**Distance (Å)**
Fe-Cl	2.42, 2.40
Fe-Cl	2.39, 2.32
C-C	1.38

Table S21. Distance between listed atoms for dissociative adsorption of cis-DCE on LC-Fe(211).

211 LC cis-DCE	**Distance (Å)**
Fe-Cl	2.33, 2.34
Fe-Cl	2.33, 2.34
C-C	1.43
C-H	1.10, 1.12

Table S22. Distance between listed atoms for dissociative adsorption of PCE on Fe(110).

110 PCE	**Distance (Å)**
Fe-Cl	2.33, 2.34
Fe-Cl	2.33, 2.34
C-C	1.43
C-H	1.10, 1.12

Table S23. Distance between listed atoms for dissociative adsorption of cis-DCE on Fe(110).

110-cisDCE	**Distance (Å)**
Fe-Cl	2.34, 2.60, 2.34, 2.80
Fe-H	1.79, 1.79, 1.78
C-C	1.38
C-H	1.10

Table S24. Distance between listed atoms for dissociative adsorption of cis-DCE on LC-Fe(110).

110 LC cis-DCE	**Distance (Å)**
Fe-Cl	2.33, 2.45, 2.42
Fe-Cl	2.38, 2.39, 2.44
C-C	1.40
C-H	1.10, 1.10

Table S25. Distance between the listed atoms (stayed in molecular form) after AIMD simulation of cis-DCE on HC-Fe(211).

Cis-DCE HC 211	**Distance (Å)**
C-C	1.34
C-H	1.09
C-H	1.09
C-Cl	1.73
C-Cl	1.73

Table S26. Distance between the listed atoms (stayed in molecular form) after AIMD simulation of PCE on HC-Fe(211).

PCE HC 211	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72

Table S27. Distance between the listed atoms (stayed in molecular form) after AIMD simulation of cis-DCE on HC-Fe(110).

Cis-DCE HC 110	Distance (Å)
C-C	1.34
C-H	1.08
C-H	1.09
C-Cl	1.73
C-Cl	1.73

Table S28. Distance between the listed atoms (stayed in molecular form) after AIMD simulation of PCE on HC-Fe(110).

PCE HC 110	Distance (Å)
C-C	1.35
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72
C-Cl	1.72

Table S29. Adsorption energy in eV of water, cis-DCE and PCE on clean, low coverage and high coverage sulfur Fe(110) and Fe(211).

Adsorbate	water	Cis-DCE	PCE
Fe(110)	-0.57	-0.51	-0.74
LC Fe(110)	-0.59	-0.42	-0.66
LC Fe(110)	-0.03	-0.44	-0.46
HC Fe(110)	-0.09	-0.43	-0.62
Fe(211)	-0.70	-1.64	-0.65
LC Fe(211)	-0.53	-0.44	-0.65
LC Fe(211)	-0.08	-0.37	-0.56
HC Fe(211)	0.22	-0.45	-0.65

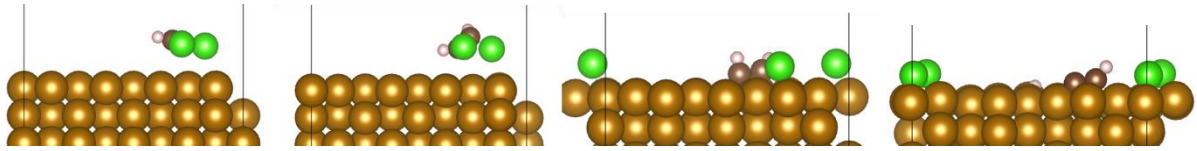

Figure S1. Snapshots of remediation process for cis-DCE on the Fe(110) surface

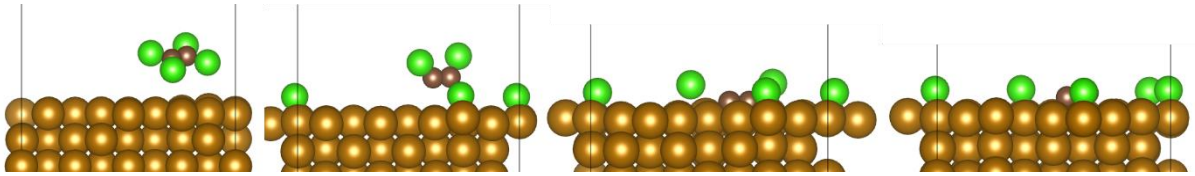

Figure S2. Snapshots of remediation process for PCE on the Fe(110) surface

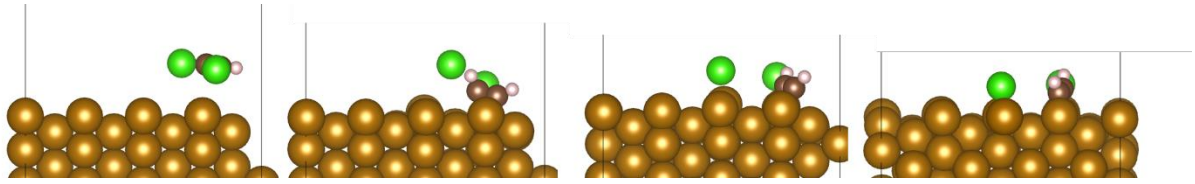

Figure S3. Snapshots of remediation process for cis-DCE on the Fe(211) surface

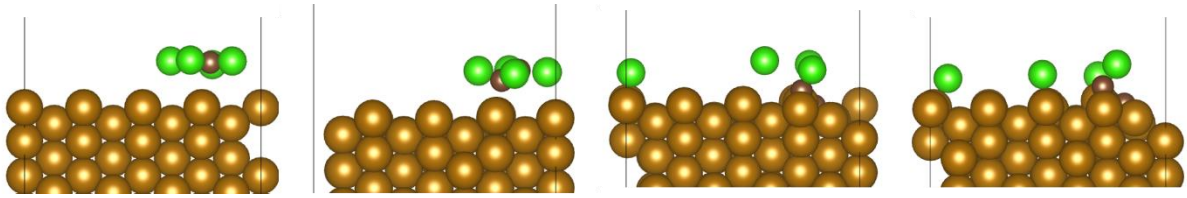

Figure S4. Snapshots of remediation process for PCE on the Fe(211) surface

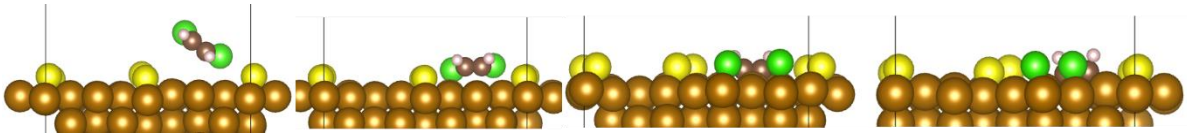

Figure S5. Snapshots of remediation process for cis-DCE on the LC-Fe(110) surface

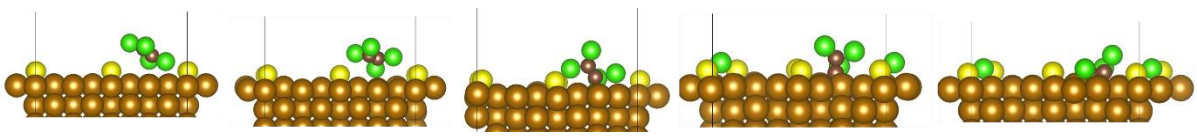

Figure S6. Snapshots of remediation process for PCE on the LC-Fe(110) surface

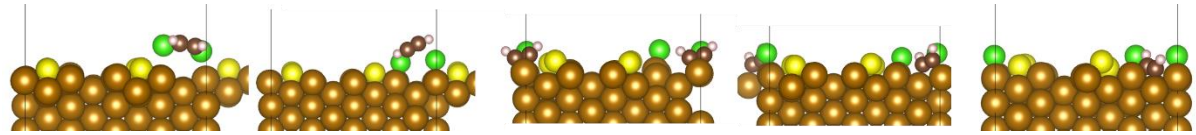

Figure S7. Snapshots of remediation process for cis-DCE on the LC-Fe(211) surface

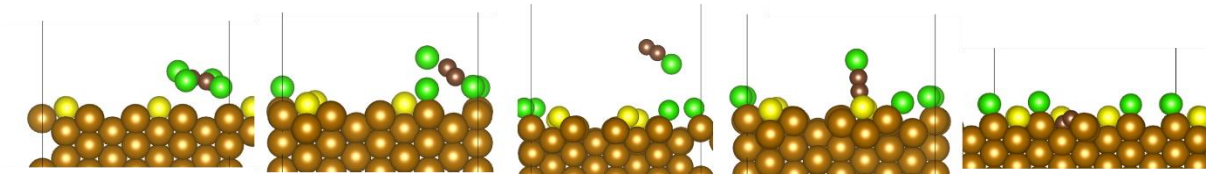

Figure S8. Snapshots of remediation process for PCE on the LC-Fe(211) surface

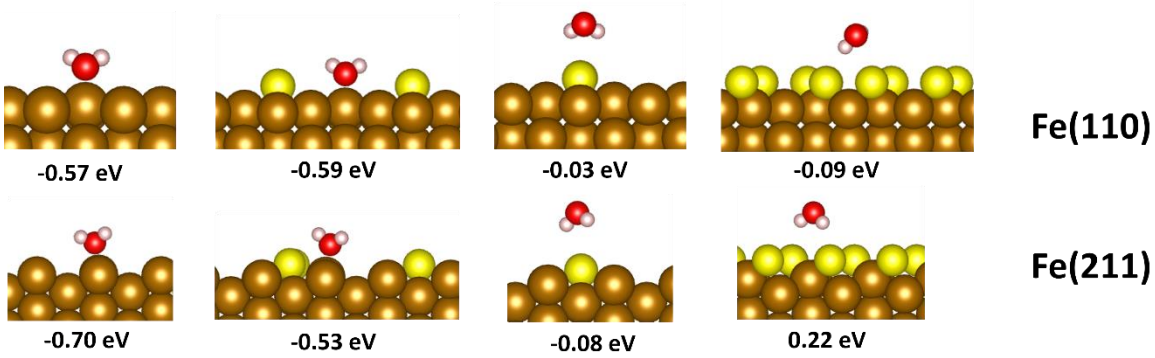

Figure S9. Molecular water adsorption on the clean, low and high coverage Fe(110) and Fe(211) surfaces