Supporting Information.

Buckingham-type interactions had the following form:

$$\varphi_{ij}(r) = A_{ij}e^{-B_{ij}r} - \frac{C_{ij}}{r^6}$$

Standard Lennard-Jones model formulation was used:

$$\varphi_{ij}(r) = 4\varepsilon_{ij}\left\{\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right\}$$

Table S1. List of Buckingham force field parameters used in simulations. The hematite crystal was kept fixed, intra-hematite interactions excluded. Water-hematite dispersion terms due to de Leeuw and Cooper [17], charges from *ab initio calculations* [20]. Modified Tsuzuki *et al* [18] applied for CO2-CO2 interactions with geometric combination rules for CO_2 and hematite.

Buckingham interactions				
Interaction	A_{ij}(kJ/mol)	B_{ij}(Å^{-1})	C_{ij}(kJ*Å^6/mol)	q(e)
O(water)-Fe	42549.82	3.0312	--	q_{Fe} =+1.31
O(water)-O(hematite)	2196380.31	6.7114	2790.34	q_{Ohem}=-0.87333
H(water)-Fe	740.680	1.8066	--	
H(water)-O(hematite)	38233.19	4.0000	--	
C(CO2)-C(CO2)	909.23	2.27	1629.9	q(C_{CO2})=0.68
O(CO2)-O(CO2)	1483300.0	4.40	1491.6	q(O_{CO2})=-0.34
O(CO2)-Fe	34967.0	2.4543	--	
O(CO2)-O(hematite)	1804962.86	5.4342	2093.9	
C(CO2)-Fe	865.73	1.7628	--	
C(CO2)-O(hematite)	44687.97	3.9032	2003.1	

Table S2. List of Lennard-Jones force field parameters used in simulations. Extended simple point charge (SPC/E) model of [7] used to model water-water interactions. Water – CO_2 LJ interactions described by potential due to Panhuis *et al* [19]. Hydrogen sulfide LJ model due to Kristóf and Liszi [29] with Lorentz-Berthelot combination rules applied to derive cross-terms for H2S and all other model components (CLAYFF force field [30] used for hematite).

Lennard-Jones interactions			q(e)
Interaction	ε_{ij}(kJ/mol)	σ_{ij}(Å)	
O(water)-C(CO2)	0.51369	3.2618	
O(water)-O(CO2)	0.81057	3.0145	
O(water)-O(water)	0.65015	3.1656	$q(O_{water})$=-0.8476
O(water)-H(water)	--	--	$q(H_{water})$=+0.4238
H(water)-H(water)	--	–	
S(H2S)-S(H2S)	2.0766	3.690	$q(S_{H2S})$=+0.4
PC(H2S)-PC(H2S)	–	–	$q(PC_{H2S})$=-0.9
H(H2S)-H(H2S)	–	–	$q(H_{H2S})$=+0.2500
H(H2S)-S(H2S)	–	–	
H(H2S)-PC(H2S)	–	–	
S(H2S)-Fe	0.00886	4.2981	
PC(H2S)-Fe	–	–	
H(H2S)-Fe	–	–	
S(H2S)-O(hematite)	1.1600	3.4220	
PC(H2S)-O(hematite)	–	–	
H(H2S)-O(hematite)	–	–	
S(H2S)-O(water)	1.2665	3.428	
S(H2S)-H(water)	–	–	
PC(H2S)-O(water)	–	–	
H(H2S)-O(water)	–	–	