Supporting Information

Title: Prediction of Hydrophobic Reagent for Flotation Process Using Molecular Modelling

Authors:

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1. Energy contributors using automatic parameters for:

1.1 4-amino-2-hydroxybenzoate

Angle Bend: (Cp C- O-) and Inversion: (Cp Cp Cp N2), (Cp Cp N2 Cp)

1.2 Erucate and Oleate

Angle Bend: (C= C2 C2)

1.3 Erucic--amino-2-hydroxybenzoate

Angle Bend: (C= C2 C2), (Cp C- O-), Inversion: (Cp Cp Cp N2), (Cp Cp n2 Cp)

2. Outputs calculated by the Monte Carlo simulation

Table S1 demonstrates outputs calculated by the Monte Carlo simulation for adsorption of different base organic ions which have hydrophobic tails in the presence of water molecules on PSM Surfaces (112) and (101)

Molecules	Scheelite Surface	Total energy Kcal/mol	Adsorption energy Kcal/mol	Rigid adsorption energy Kcal/mol	Deformation energy Kcal/mol	Base Organic ions: dEad/dNi Kcal/mol	Water : dEad/dNi Kcal/mol
Oleate and water	112	-2017.23	-2060.54	-2191.26	130.72	-499.38	-81.87
		-2016.08	-2059.39	-2191.36	131.97	-497.80	-81.82
		-2015.37	-2058.68	-2188.63	129.95	-495.41	-83.75
		-2013.05	-2056.36	-2202.12	145.76	-492.37	-79.32
		-2012.39	-2055.70	-2185.65	129.95	-493.21	-82.61
		-2012.08	-2055.39	-2183.20	127.80	-492.73	-82.64
		-2011.78	-2055.09	-2185.22	130.12	-490.84	-82.67
		-2010.44	-2053.75	-2184.21	130.45	-490.41	-81.34
		-2009.56	-2052.87	-2176.52	123.65	-490.07	-80.64
		-2008.33	-2051.64	-2191.83	140.19	-487.89	-79.28
	101	-3381691.00	-3381735.00	172467.80	-3554202.00	182865.80	-8354.94
Erucate and water	112	-117997.10	-118043.30	-905.20	-117138.10	-110486.10	5.40
	101	-182260.80	-182307.00	241.57	-182548.60	-139380.50	91.23
4-amino-2-hydroxybenzoate and water	112	-11088110.00	-11088140.00	1566152.00	-12654290.00	654856.70	-134077.00
	101	-2492.24	-2520.69	-2637.10	116.41	-320.41	-127.45
		-2483.43	-2511.88	-2628.91	117.03	-327.88	-126.64
Erucic-4-A 2-HB and water	112	-222517.10	-222598.30	1284.97	-223883.30	-180437.00	460.49
	101	-2820.70	-2901.90	-3134.28	232.37	-1159.87	-112.41
		-2814.11	-2895.31	-3109.88	214.58	-1186.99	-107.37

2.1. Final Steps of Monte Carlo

The calculated energy and interaction energy were tabulated for each system at final step of Monte Carlo (2.5*105). In addition, minimum adsorption energies in Table S1 are reported in Table S2.

Table 2, Final steps of MC during liquid-solid interface and minim adsorption energies for different hydrophobic reagents on the PSM surfaces (112) and (101).

Liquid and Solid Surface		Total Energy Kcal/mol	Average Total Energy Kcal/mol	Electrostatic Energy Kcal/mol	Intramolecular Energy Kcal/mol	Interaction Energy Kcal/mol	Average Interaction Energy Kcal/mol	Average Adsorption Energy Kcal/mol
Oleate and Water	(112)	-1660	-1570	-1680	43.3	-1710.9	-1912.05	-1691906.77
	(101)	-2070	-2030	-2090	43.3	-2113.2		
Erucate and Water	(112)	-1710	-1600	-1770	46.2	-1758	-1878.75	-150157.15
	(101)	-1950	58000	-2060	46.2	-1999.5		
4-A-2-HB and water	(112)	-1980	-1740	-1900	28.5	-1914	-2109.405	-2206.215
	(101)	-2280	-2170	-2300	28.5	-2304.81		
Erucate-4-A-2-HB and water	(112)	-1830	1250	-1870	81.2	-1916	-1080	-112750.1
	(101)	-2200	-2150	-226	81.2	-244		

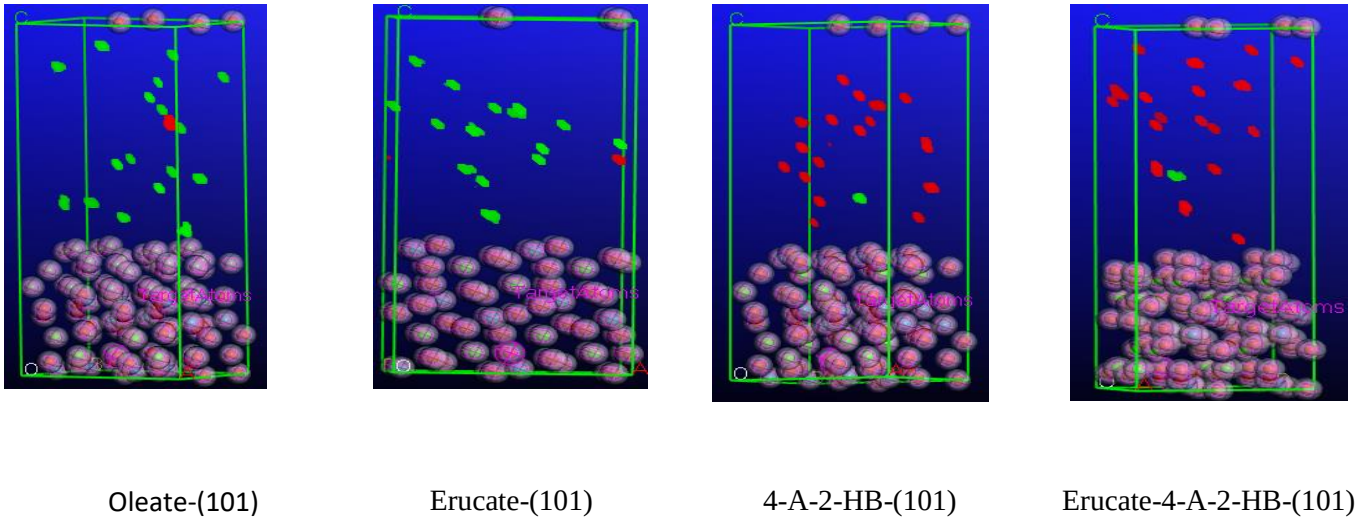
2.2. Rotation and Translation Steps

Intramolecular degrees of freedom have been considered for base organic ions and water molecules during liquid-solid interface, as a motion group, and ratios between, total rotations or translations accepted and total rotations or translations attempted are given in Table S3.

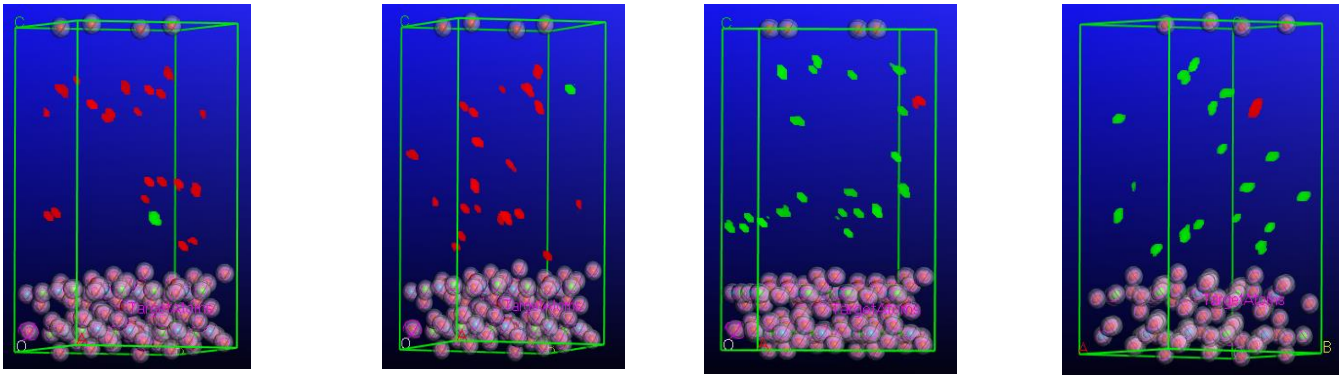
Table S3 Monte Carlo rotation and translation steps for base organic ions and water molecules on the PSM Surface s (112) and (101)

molecules	Ratio between accepted and attempted				PSM Surface
	rotation steps	Average rotation steps	translation steps	Average translation steps	
Erucate-4-A-2-HB and water	0.455	0.4365	0.079	0.076	112
	0.418		0.073		101
Erucate and water	0.328	0.389	0.087	0.0775	112
	0.450		0.068		101
Oleate and water	0.498	04905	0.081	0.0805	112
	0.483		0.080		101
4-A-2-HB and water	0.502	0.503	0.093	0.086	112
	0.504		0.079		101

Calculations have demonstrated that molecules contain only aromatic compound or carboxylate ions have high mobility on the PSM surfaces (112) and (101) due to low interaction energy, whereas molecules contain mixtures from an aromatic compound and erucate have low mobility on the PSM surfaces (112) and (101) due to high interaction energy.



Oleate-(101) Erucate-(101) 4-A-2-HB-(101) Erucate-4-A-2-HB-(101)



Oleate-PSM(112) Erucate-(112) 4-A-2-HB-(112) Erucate-4-A-2-HB-(112)

Figure S1 shows adsorption density fields during the interaction between based molecule ions and PSM surfaces (112) and (101)

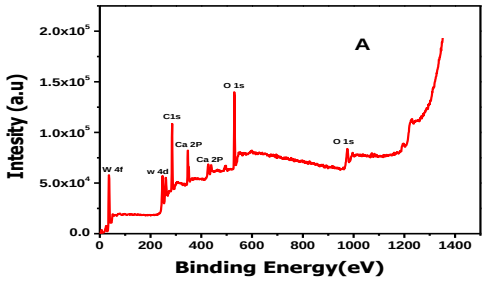


Figure S2, binding energy of atom orbits on mineral surfaces after adding sunflower Soap.

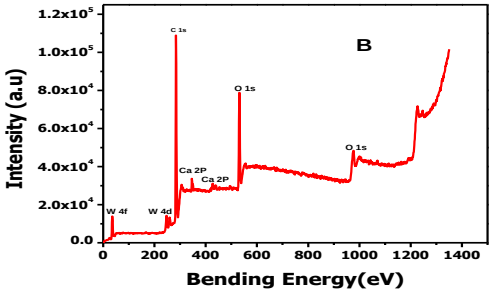


Figure S3, binding energy of atom orbits on mineral surfaces after adding mustard Soap.

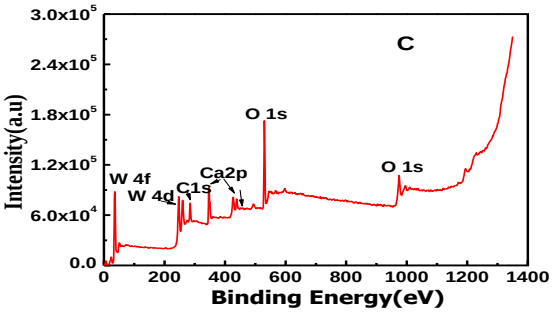


Figure S4, binding energy of atom orbits on mineral surfaces before adding sunflower or mustard Soaps.

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Professor Peng got his ph,D. from Wuhan university of Technology in 2005, his research interests, include mineral processing of metallic ores and waste treatment of solid and liquids and he is supervisor of the current projects.

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