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Supplementary information for

**Interfacial Adsorption Mechanism of Diethyldithiocarbamate in  
High-Sulfur Residue Flotation**

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**The SI contains two figures, one table, and one text section.**

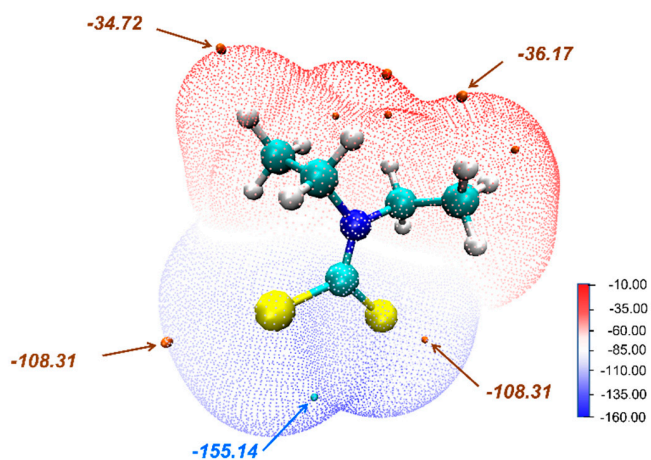


Figure S1. Electrostatic potential distribution of DDTC.

Gaussian parameters: m062x/6-311++g(2d,p), em=gd3, scrf=(solvent=water,iefpcm)

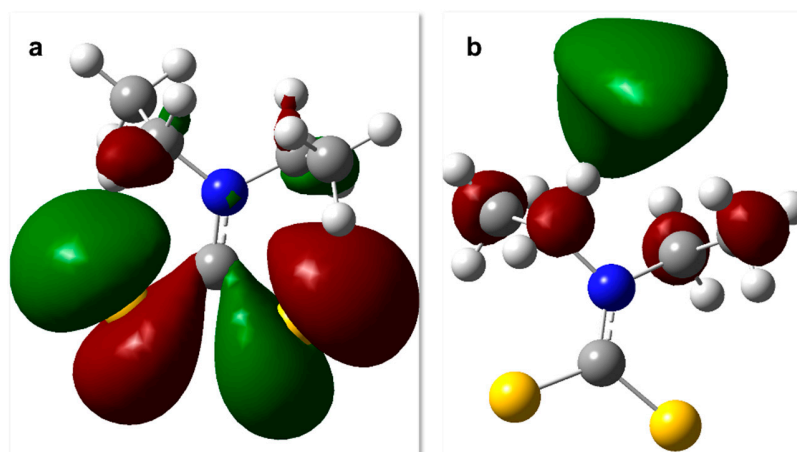


Figure S2. (a) HOMO orbitals of DDTC; (b) LOMO orbitals of DDTC.

Gaussian parameters: m062x/6-311++g(2d,p), em=gd3, scrf=(solvent=water,iefpcm)

Table S1. INCAR file for VASP optimization process.

INCAR	Keywords	Parameters
Basic parameters	ISTART	0
	ICHARG	2
	ISPIN	1
	ENCUT	400
	PREC	Normal
Electronic relaxation	ISMEAR	0
	SIGMA	0.05
	NELM	200
	NELMIN	3
	EDIFF	$10^{-5}$
Ionic relaxation	NSW	100
	IBRION	2
	POTIM	0.5
	ISIF	2
	EDIFFG	-0.05

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## Supplemental DFT Calculation Information

### S1. Electrostatic potential and frontline orbit of DDTC (Related to [Figures S1 and S2](#))

[Figure S1](#) shows the electrostatic potential on the surface of DDTC. The sulfur atom in the polar group was the region of negative potential concentration of DDTC. An electrostatic potential minimum of the DDTC existed in the middle of the two sulfur atoms (-155.14 kcal/mol). Two extreme points of electric potential existed around the two sulfur atoms (-108.31kcal/mol), which were symmetrically distributed. This meant that the sulfur atoms in DDTC were more likely to adsorb on the surface of the mineral phase.

[Figure S2](#) shows the HOMO and LOMO orbitals of DDTC. The HOMO was mainly composed of sulfur atoms in polar groups, and the LOMO was mainly composed of two ethyl groups. In the flotation process, the collector usually acted as the electron donor, and its HOMO orbitals usually transferred electrons to the mineral surface. Therefore, the sulfur atom in DDTC was the active site for chemisorption.