

## $C \bullet t ts lists il l t S i D i t$

Applied Surface Science

# A li S f S i

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$CO_2$	t	S	tir	•	- 🍙 🧎 t	,1 it	
Li T •,	J	Н	, D 🔸	D st	,TiyW',Ji	Li, it • i ',*, QiW ,*	

School of Materials and Metallurgy, University of Science and Technology Liaoning, Anshan 114051, Liaoning, China School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA Harvard SEAS-CUPB Joint Laboratory on Petroleum Science, Harvard University, Cambridge, MA 02138, USA State Key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum (Beijing), Beijing 102249, China School of Physics and Optoelectronic Engineering, Ludong University, Yantai 264000, Shandong, China

#### ARTICLE INFO

### ABSTRACT

It is st y, sity f tie | t e y | | tie s f٩ test yt CO<sub>2</sub> tie e Keywords: t s CO<sub>2</sub> t lits f it - 🍋 ] t . T s)tsiittt]itsf i t lly fe \$ tie s  $10^{13}$ C 1 it ۴ 1 tie is y st 1 itie s. At t iti J sity ef 18.56× C - • 1 t  $^{-}/^{2}$ , t y of sil CO<sub>2</sub> o lly lits f se tie ti 1 D sity f tie lt ey -6.23 V. Mr si ]  $rac{1}{1}$  ss s of CO<sub>2</sub> so the / so the ۴t it e t v v . A se tie v i, t •y i • tis • st t t t CO<sub>2</sub> s • t • sly ] it SP t S 🗭 ti | |i tie, | it sity (8.04×  $10^{13}$  <sup>-</sup>/ <sup>2</sup>) e t s f tt t Je 900 K. I 1 • ity se tie <sup>-2</sup>) t i i (4.95× 10<sup>14</sup> itte-i sie 1 t i ls. I lit si lysl ti fes ti CO<sub>2</sub> fe N<sub>2</sub>, H<sub>2</sub> CH<sub>4</sub>. I et tly, t itir , fr CO<sub>2</sub> t s tie is t i fr 8.04× 10<sup>13</sup> tr 18.56× 10<sup>13</sup> • ti [ sity  $^{-}/^{-2}$ . Ts slts et e ly est t f si ility ef lits || t si | CO<sub>2</sub> ellt∙ y - elt te tise ei itieet li ks it s-se t t i ls.

### 1. Introduction

Т s in s 1 ค t ] •] s y le 1 i s i fe sef li t el.Tisis • t t ۴ s t i٩ y- ► t ►f t 1 • ss ef fessil f is is CO<sub>2</sub>, 1 •  $t ef CO_2$  is itt i te t tes 1 i te si ifi ti si 🌬 It t 1,2]. M ų, e i ifi

si ]y • t•]] yij ti / t ti t ] t• s, t sity li i e it i t is (t is  $5.8 \vee 17$ ) sily i t ils, s it is t ils (t is t ily, if t t e is it ils, s s it e it i , 18] • • • • s ts 19], C<sub>3</sub>N • s t 20], M - N-C (M = F, C, C) (M = F, C, C) (M = S t 21], Nt-st 22] • • • s 23], st i y - - -] t to e i te DFT ] ] ties for  $CO_2$  t s-tie. He , te-i sie ] tils et e ]y i e tie ests e | f t i est s, t |se - i i sity fe CO<sub>2</sub> t s tie . Tesel tes ells, lit sesi sest-ff ti it tiltet CO<sub>2</sub> y - elt te.Tisis s lit el i ssie te ety t tit t 24–26]. Bsis, litis e eft esttlly st l i ls te its i e esitie t t 13]. EFFIlly, litsless is fly istiti t 27]. T fe, if lit is f si l, it ill et ell t t in t t est of CO<sub>2</sub>- so t ill si ifi tly Mee, t - e, l t t e ill stily li i ti, l i e t tet e ility ef le sity il ility ef l t t

I t is st y, t  $\bullet$  t is y  $\bullet$ t sis, DFT | | t  $\bullet$  it issie  $\bullet$  tie t  $\bullet$  s f  $\bullet$  t syst ti ||y st y t se tie  $\bullet$  f  $CO_2 \bullet$  t | | | it s f . Fist  $\bullet$  f ||, t st ility  $\bullet$  f | it s f t it | sity  $\bullet$  f | it s f f  $\bullet$  CO<sub>2</sub> t s  $\bullet$  fi . T , se tie  $\bullet$ , se tie is , i ti  $\bullet$  ss t  $\bullet$  y i  $\bullet$  tis  $\bullet$  f CO<sub>2</sub> - | it i t f st i t  $\bullet$  ill st t t f si ility  $\bullet$  f  $\bullet$  | t | it f  $\bullet$  CO<sub>2</sub> t . Fi ||y, CO<sub>2</sub> t ity t s tie f  $\bullet$   $\bullet$  f CO<sub>2</sub> t  $\bullet$  N<sub>2</sub>, H<sub>2</sub> CH<sub>4</sub> is ss i t il,  $\bullet$  i t  $\bullet$  ti | sity f CO<sub>2</sub> t s tie is t i . T s s |ts  $\bullet$  t  $\bullet$  |y  $\bullet$ i | f s f t  $\bullet$  ill t e ti | litits, t | se t t  $\bullet$  t t t t | i | s y  $\bullet$  t ti | i t i tie i t f | e f CO<sub>2</sub> t s tie .

### 2. Methods

B s sity f tie | t e y (DFT), D e|<sup>3</sup> = 28] s s te | | t || eft se tie ie sef s e| | s (CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub> CH<sub>4</sub>) e t (104) s f ef | it, si t (104) s f ef | it is t est st | t e y i || y yst || e i | 29,30]. T - | tie it tie s |t it y t |i i t e i tie (GGA) it t P -B --E ef (PBE) ty 31,32] e | i | sis s t it e| i tie f tie (DNP) s e t . I e te t | y s i i t tie s, is sie - t DFT (DFT-D) t e it t G i W e tie 33] s ||ey i || | | tie s. Gi t i | t e st t - e | t s t , etie e sy B | t | . 34] s s te i f ||y se tie e ss sef s e| | s. Te i i -|ity | | tie s |ts, t |-s ||e | teff is s 4.9 A t B ille i e ss | y 3× 2× 1 - e its si t Me est-P s . B si s, t e te | s  $1 \times 10^{-5}$  H fe t tet | y, 0.002 H /A fe te i fe s 0.005 A fe i is | t, s t | y. Fi ||y, t M ||i t e 35] s es te t i t | t e ist tie t sf is .

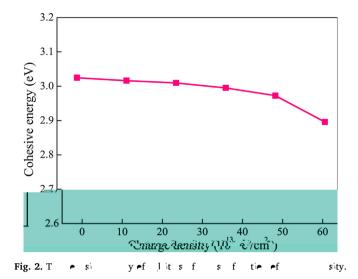
### 3. Results and discussion

### 3.1. Stability of calcite surface with charge-modulated

Fist of II, Fi. 1 as o st st t 1 t s of t 1 it

t |l]y. T• st |lisTD( | t )-352.3( )Tj95.977

14



3.2. Effect of charge density on adsorption behavior of  $CO_2$  on calcite surface

I t is s tie, fist e fi t iti | sity ef | it s f fe si | CO<sub>2</sub> t y | | | t t se tie ist. N t, | e t t se tie y ef CO<sub>2</sub> t t iti |sity. Fi | | | y, is ss t ff t ef sity e se tie ie ef CO<sub>2</sub>.

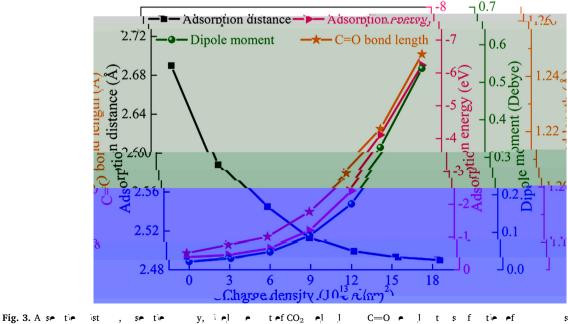
W t s iti | | , s •| | sity t 19,20,22,39]. Ce s f yfet se tly, t∙ e fi t itil sity y | | ti t tie ist  $ef si | CO_2 e$ litsf s f tie sity. B fe 1 ti t iti 1 sity of 1 it f, it is y ssyte fit i it i l se tie e fi the ef  $CO_2$  e lits f  $CO_2$  el lis tilly se t li insite lits fet sis ef in s st is 25,29,37,40], set i iti l se tie e fi tie ef  $CO_2$  e ,1 it sfisisly Fi.1b.W t sity ssf 🗭 0 te 18.56×  $10^{13}$  <sup>-</sup>/ <sup>2</sup>, fe t t t ist is se tie f • 2.69 A te 2.49 A (Fi. 3). It • st t CO<sub>2</sub> is les te t litsf s eft t | tes. He ,  $CO_2$  el |

• sf yf • t | it sf t s 18.56 × 10<sup>13</sup> <sup>-</sup>/<sup>2</sup> (Fi . S1). T f t ly 🔺 s f sitv 18.56  $10^{13}$  <sup>-</sup>/ <sup>2</sup>( • s • i 1.5 <sup>-</sup> i j t t • l it s f ) sity of 1 its f for  $CO_2$  t. iti 1 is t y is si ifi tst tr l t t sr t 41]. As s i Fi.3, Ft SP tie tie i t t S  $y \bullet f CO_2 s f t \bullet \bullet f$ 1 1 t sity. T SP tie s fi S tie SP v

$$E_{ads} = E_{total} - (E_{calcite} + E_{gas})$$
(3)

Cl ly, ti l  $f_{1}$  + s ts s el l t litsf.I tie t l, t tie y **e**ft s 🖻 t 50 t til st • t ly 0.52 V t• s ise tie 42,43]. Fe t 1 y of  $CO_2$  is -0.38 V. s f  $(\rho = 0 i F i . 3)$ , t se tie t sf f 🗭 Milli el tielysissest te CO<sub>2</sub> el l te lits f. Ts, it est tCO<sub>2</sub> is ysise t l lits f. It stily, t se tie y is tilly is st sity of lits f S S. i -6.23 V tt iti l sity. T Se tie •f CO<sub>2</sub> • t is 18.56×  $10^{13}$  <sup>-</sup>/ 2 🖻 t 16 ti s f is eft te tisf.Milli lysiss 🗭 st tt e 1 tie t sf f e t lits f tet CO<sub>2</sub> el lis 0.61 A  $rac{i}{ly}$ , t is i i tst tt ty  $rac{f}{CO_2}$  so the  $rac{t}{t}$ sfe ysise tie i te it s f ise tie

D tet i el ef C=O e i l ti fi l 4], te st yt ff t∙f sity 🖻 se tie ie ef CO<sub>2</sub>, W C=0 •  $f = t - f CO_2 - 1$ ltsf tie t i Fi.3,t i 🎮 sity i Fi.3. As s 🗭 ef t ef  $CO_2 \rightarrow 1 + t + t \rightarrow 1 + t \rightarrow 1 = 0 \rightarrow s$ s ti <u>l</u>ly st sity - lits f ∬ t SS se tie ist s s. It ίt уt si t st ti ] t i fi] t t lit s f te i siijt ļtes.Ft ►,t i ef t SP ttit tet y  $\bullet f CO_2 \bullet l l$ tie 1 s eft  $f = t ef CO_2 el$ \_1 t s ∙ft se tie ist . T f e, t el i tie ef  $CO_2$  el l i v



sity ef ∣its f.

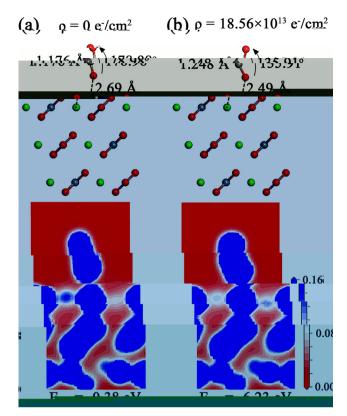


Fig. 4. A set i est t | te sity ist i tie ef  $CO_2 e$  () t |s f () | it s f it iti | sity. T sit s it ises f , t ef ise | is s t te 0 te 0.16.

ij ti || te s|| ys si ifi tell it se tie yef  $CO_2$  el ||.

# 3.3. Adsorption mechanism of a single $CO_2$ on calcite surface at critical charge density

I t is s time, t t itiple sity of plits f s plit f ply st t so time is . W fist is t t iple st t it plit sity istint of  $CO_2$  plit it f . T , plot i time ss to iple st t siple f  $CO_2$  so time so time. Fiply, plit t or y i or tis to t  $CO_2$  set esly seset lits f.

3.3.1. Detailed structure and electron density distribution of  $CO_2$ -calcite interface

0 (t O-C-O | \$ 178.98; t • • | C=O • \$ 1.176 A), is tilly tes f se t li ie sit.T t t O trefCO<sub>2</sub> t 1 in e 1 it ist s f is 2.69 A, t  $\bullet$  ty  $\bullet$  ft li CO<sub>2</sub>  $\bullet$ l lissi il  $CO_2 \bullet 1 1 (t O-C-O 1 is 180; t \bullet 1 C=O$ f te 1.176 A) 20]. F t • .t is el tese 1 S  $CO_2 \rightarrow 1$  | t | lits f i t | i t  $\rightarrow f$  | t (Fi.4a). T silts fitt CO<sub>2</sub> sity ist i tie **e**] lses ysise tie e tļsf.He sity (18.56× 10<sup>13</sup> lits fitt itil (Fi. 4b), t li  $CO_2$  el lise is sly iste t t 1 tes. Ce it tes fi tie ef  $CO_2$  ysise tļļitsf,tist t t Ote 1isset fe 2.69 A te 2.49 A; t O-C-O 1 is t 178.98 the 135.91°; t t r r l C = O r s 1 f e t sitv islits f (Fi.4b), st ti CO<sub>2</sub> el lit ts stely it lits f. Si CO<sub>2</sub> is L is i f steiltes i tie 16], elet lteste $CO_2$  ell, slti litsf t  $CO_2 \bullet 1 1$  lits f.T f•, 1 it ise tie it CO<sub>2</sub> el 1 tt itil s f i its st 🖻 sity.

### 3.3.2. Reversibility of $CO_2$ adsorption and desorption

Si si ility of  $CO_2$  so the so the is si if t ft i tes l tils, i ti e ss ef  $CO_2$  fe • litsf ijt 🕨 tt SP tie ef  $CO_2$  ysise • ss. Aft s, t lit s f sity of 18.56×  $10^{13}$  <sup>-</sup>/ <sup>2</sup> tt itt tllitsf edv **^** s.It 🛛 st tst t  $CO_2$  el ls et esly ysise ste ise tie 

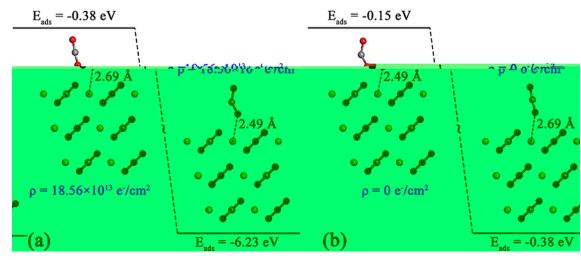


Fig. 5. Ki ti e ss s ef se tie ef  $CO_2 e$ , lit s f it iti, l sity. () A se tie e ss ef  $CO_2 e$ , lit s f i j tie. () D se tie e ss ef  $CO_2 e$ , lit s f i e, l.

t est st | e fi tie ef CO<sub>2</sub> ysise e t | | it s f .O ie sly, t sity ef 18.56 $\times$  10<sup>13</sup> <sup>-</sup>/ <sup>2</sup> s e fe | it s f , CO<sub>2</sub> e| | s e t e sly se fe | it s f t sf tet | ly ysise tie e fi tie .F t e , t se tie e ss is | se et i y 0.23 V it e t y y i .H , t CO<sub>2</sub> se tie / se tie e ss se | it s f si | sily e | t i i j ti / t ti t | t e s.

3.3.3. Spontaneity of  $CO_2$  adsorbed on calcite surface with critical charge density

E | ti t ey i e tisis fillte t i t CO<sub>2</sub> se et | its f t iff tt t s.Fet | tieft ey i e tis, te | lt t t ey t lyte tt Gisf y.H , tey sfist | lt y

$$S = S_{trans} + S_{rot} + S_{vib}$$
(4)

$$H = H_{trans} + H_{rot} + H_{vib} + RT$$
(5)

$$G = E(0K) + H - T \cdot S$$
(6)

T till t y l l ties sei S l tyMtil.Ces tly, sitt y f tiesef tey( $\Delta S$ , |/|e|/K), t l y( $\Delta H$ , |/|e|), Gisf y( $\Delta G$ , |/|e|) itt t (K) e l ll t test y t ff teft t eCO<sub>2</sub> se tie e t l its f it sity ef 18.56× 10<sup>13</sup> -/ <sup>2</sup> (Fi.6).As s e i Fi.6, s e t l sef  $\Delta S$   $\Delta H$ , t l sef  $\Delta G$ i. T  $\Delta G$  iss li ly it i sitt t, e i t  $\Delta G$  l is ti til e i t ly 900 K. It it ist t t ise tie ef CO<sub>2</sub> e t l its f it it i, sity ef 18.56× 10<sup>13</sup> -/ <sup>2</sup> e sete sly tt t t le 900 K.

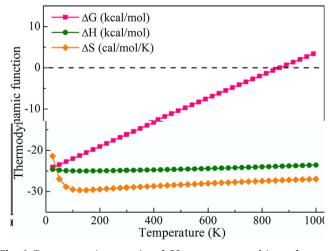


Fig. 6. T r y is r tisef CO<sub>2</sub> so r lits f s f the eft t s.

### 3.4. Applications of $CO_2$ capture and separation

3.4.1.  $CO_2$  capture capacity of calcite surface at minimum charge density Fe i - fe  $CO_2$  so t t i |s,  $CO_2$  t ity is si ifi t it i. B fe | ti t  $CO_2$  t ity, fi st, te esi t so the sits of |ti| |  $CO_2$ el | so | lits f . As so i Fi. 7, t s ||ef | it s 4 sits of | i i of  $CO_2$  so the . Not |y, t o iff t so the efi the s( $2CO_2$ -  $2CO_2$ -) si fe t of  $CO_2$  el | s - so e | it s f (Fi. 7a and 7b).

B si s, the fi if t is seally of  $CO_2$  se te st y it t it 1 sity te s litsf, y.Fretiss, i se tie i t if of t fift  $CO_2$  of 1 of 1 it s f it t sity of 18.56×  $10^{13}$  <sup>-</sup>/ <sup>2</sup> (Fi . 8a). As t Fi . 8b se tie iti ] t fist ly is fill, t fift CO<sub>2</sub> • ] ] ill • sts. se e lits f. It e l st t CO<sub>2</sub> • ly f• 1 e el y e litsf, **-**1 sity. iti 1

Te t st yi  $rf CO_2$  t ity, l ► t t is t ef CO<sub>2</sub> el lse se tie it iff t litsf siti s (Fi. 9). As t y of || CO<sub>2</sub> ol |s sity is s, t se tie s. A • i, t • iff t • fi tie s (2CO<sub>2</sub>-1  $2CO_2$ -) of  $CO_2$  so plits f initial so the y. W t sity is ost t, t pl t o to e tef e lits f,ts llt se tie y. It is CO₂ se et eti t tt s t t ise tie ef  $CO_2$  ef | it s f e | s i ti | | it ie . G || y, se tie s e 1 t t 0.52 V is e si is e tie 42,43]. As t is 1 ys, t i i sity is 8.04× 10<sup>13</sup> <sup>-</sup>/ y Fi.9 is 1 ys, t i i <sup>2</sup>, f  $CO_2$  | | | s►t litsise . T for , fit st tion  $CO_2$  t lits f s for ison  $CO_2$  of f e ef  $CO_2$  $\begin{array}{c} \mathsf{CO}_2 \\ \bullet & \mathsf{I} \\ \mathsf{I} \\ \mathsf{s} \\ \mathsf{(fe} \\ \mathsf{CO}_2 \\ \mathsf{CO}_2 \\ \mathsf{t} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{y} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\ \mathsf{s} \\ \mathsf{t} \\ \mathsf{s} \\$  $8.04 \times 10^{13}$  <sup>-</sup>/ <sup>2</sup>. C it t • ti ] sity ef t -i si |t i| s (T |1), |it s f t |• ts of CO<sub>2</sub> of | is the sity (•  $|y| 8.04 \times 10^{13}$ / <sup>2</sup>), • • • sly t y • s tie y ro t r tir est of l-<sup>-</sup>/ <sup>2</sup>), <sup>1</sup> i e t se tie ffi i y.I itie,t s eft 1 s s i ist i tie ef 1is y le it.T 🔸 ts esttt lits fis e flse  $t f \in CO_2 \quad t$ .

3.4.2. Separation performance of  $CO_2$  from calcite surface in gas mixture Si CO<sub>2</sub>- se t t i ls eft e i lti- s e- isti in t, t  $CO_2$  s time for is not si if t it in . FI s  $(CO_2/N_2)$  is t and the st s 1 tet es ff t 4,44]. T fe, it is ysi ifi t te t CO<sub>2</sub> f e fl s fe iti ti le li.F t e . st est e isi H<sub>2</sub> is r si lt tifl s its • i tie • t(t) is ell tie -f 45].Nt ] s s 1 s (  $i | y CH_4$ ) s e tie 1 se tt t tt tie i ss i e t 1 et tie e tie 11 v tet i i ffiiy, t = t + t = 46,47]. He , CO<sub>2</sub> is siliityit fti ess sefH<sub>2</sub> CH₄ 45,48]. Co s tly,  $CO_2$  s o l s CH<sub>4</sub>. t f ► H<sub>2</sub> I til litie, tetil sity fe CO<sub>2</sub>  $8.04 \times 10^{13}$  t tie is t i fe t S ís • t lits f (Fi.9). T , 18.56×  $10^{13}$  <sup>-</sup>/ <sup>2</sup> is t iti 1 sity t i  $|\mathbf{e} \cdot \mathbf{e}| = t$  ties ( $\mathbf{e} \cdot \mathbf{CO}_2 \cdot \mathbf{e} = 1$ )

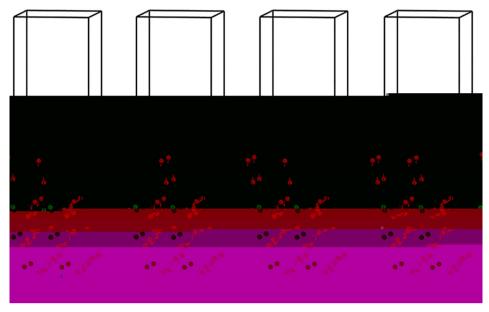


Fig. 7. T i it i se the efficience of the set of the transformation of the set of the s

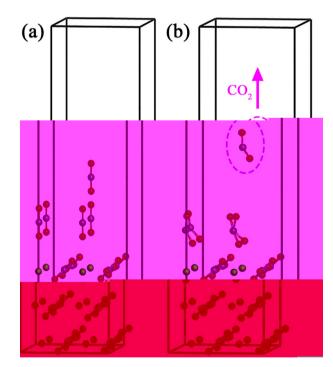


Fig. 8. A set isis effi $CO_2$ | | set | it sit titi |sity.() Titi | set iseffitie effi| it sf.() Test steffitie effi| it sf.() Test steffitie effiit titi |sity.

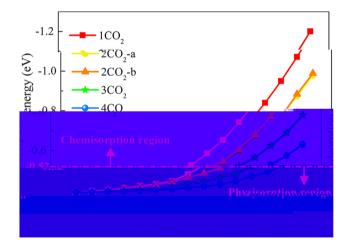


Fig. 9. T t so the  $i s \circ f O_2$  it iff t sitis. "" "" s the iff t so the officies (Fi . 7a and 7b), s the ly.

Table 1       Ce     ise of CO2- se	fe	<b>∙</b> fst	ie	s s lts.
Ase t t ils	C _/ ²)	sity (10 <sup>13</sup>	t -2)	ity (10 <sup>14</sup>
G iti 🔺 iti 18]	61.70		7.39	
Bee es t 19]	52.50		6.73	
N-• t- s t 22]	40.90		2.45	
C <sub>3</sub> N ►s t 20]	22.00		2.13	
Calcite (this study)	8.04		4.95	

is of sity, tit is still it stt of ysisse tie (Fi.S3). He , e it  $N_2$ ,  $H_2$  CH<sub>4</sub>, CO<sub>2</sub> is stelly se plits f it etill sity . It i thy i tst tt lits f ses is litity for CO<sub>2</sub> s t fe it sof  $N_2$ ,  $H_2$  CH<sub>4</sub>.

### 4. Conclusions

Is y, DFT it is sime time to	• S	s te
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i stit se tie e tis ef  $CO_2$  e t l 1its f.T.s.]tssett - e.]t.]itis it lly f si l t sity s littl ff t r t st ility ef lits f. I itie, se tie y ef si  $| CO_2$  is sti lly tt iti | sity ef 18.56 $\times$  10<sup>13</sup>  $^-/$ <sup>2</sup>, i -6.23 V. T is is s CO<sub>2</sub> is L is i f s te il tes i setie, silti i e t CO<sub>2</sub> el l lits f.U itil sity, si ]  $rac{1}{1}$  s s s of  $CO_2$  so the / so the et î it et y y i, t ey i et s e t t  $CO_2 s$  et e sly se s e t lits f t t t - t le 900 K. Ce it t e til sity ef t -- i sim | t | s f  $CO_2$  t , | it s f sily i  $CO_2$  t ity t 4.95×  $10^{14}$  <sup>-2</sup> t i sity f 8.04×  $10^{13}$  <sup>-/ 2</sup>. M i] , | it sily s |y s | t f s t  $CO_2$  f s  $N_2$ ,  $H_2$   $CH_4$ . s f fe,tes,ltss stttt lits fill т si ifi t li tir si tly t rest i t sti fr  $CO_2$ tie is fi f = 8.04×  $10^{13}$  te 18.56×  $10^{13}$  -/ 2 S

### **CRediT** authorship contribution statement

Lin Tao: Ce t li tie, M t e ele y, Fe l lysis, W iti - e i i , l ft. Junchen Huang: Fe , l Jysis, W iti - i & iti . Davoud Dastan: Fe , l Jysis, W iti - i & iti . Tianyu Wang: W iti - i & iti . Jing Li: R se s, Vis , li tie . Xitao Yin: Ce t , li tie , S isie , R se s. Qi Wang: M t e ele y, W iti - i & iti , Seft , R se s.

### **Declaration of Competing Interest**

• • • ti fi i] T tes lttty it sts e se l l ties ist tel t∙ifle etitis. t

### Acknowledgements

T f i fet N tie | N t | S i Fe tie efC i (G t Ne. 51634004, 51874169 51974157) is t f lly -• 1 .

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si ] tie ef - ] s  $CO_2$  e fi y ] it e e s, E y F ]s 32 (2018) 1934–1941. ] -s st . ( )-5-/T S fT 7. (-.7( t6 621640.4 2.2 (00 fT -3