

Electronic Supplementary Information

A DFT-based microkinetic study on methanol synthesis from CO₂ hydrogenation over the In₂O₃ catalyst

Zhimin Zhou,^{a,b} Bin Qin,^{a,b} Shenggang Li,^{a,b,c,*} and Yuhan Sun^{a,b,c}

^aCAS Key Laboratory of Low-Carbon Conversion Science and Engineering,
Shanghai Advanced Research Institute, Chinese Academy of Sciences, 100
Haik Road, Shanghai 201210, China. E-mail: lisg@sari.ac.cn.

^bUniversity of Chinese Academy of Sciences, 19 Yuquan Road, Shijingshan
District, Beijing 100049, China

^cSchool of Physical Science and Technology, ShanghaiTech University, 100
Haik Road, Shanghai 201210, China

Emails: lisg@sari.ac.cn

Table S1. Elementary reactions considered for CO₂ conversion to methanol on c-In₂O₃ (110) and (111) in microkinetic analysis performed with CatMAP. To simulate the CO formation rate of the CO-O route in Fig. 1, the elementary steps of the COOH pathway will be replaced by the elementary steps of the CO-O route.

R1	CO ₂ _g + *_s -> CO ₂ *_s
R2	H ₂ _g + *_t + *_v <-> H-H*_v + *_t -> H*_t + H*_v
R3	H ₂ _g + *_t + *_t <-> H-H*_t + *_t -> 2H*_t
R4	CO ₂ *_g + H*_t + *_s <-> H-COO*_s + *_t -> CHOO*_s*(mono-HCOO*) + *_t
R5	CHOO*_s -> HCOO*_s(bi-HCOO*)
R6	HCOO*_s + H*_t <-> H-HCOO*_s + *_t -> H ₂ COO*_s + *_t
R7	H ₂ COO*_s + *_s <-> H ₂ CO-O*_s + *_s -> CH ₂ O*_s + O*_s
R8	CH ₂ O*_s + H*_t <-> H-CH ₂ O*_s + *_t -> CH ₃ O*_s + *_t
R9	CH ₃ O*_s + H*_v -> CH ₃ OH*_s + *_v
R10	CH ₃ OH*_s -> CH ₃ OH_g + *_s
R11	H ₂ _g + O*_s + *_t <-> H-HO*_s + *_t -> OH*_s + H*_t
R12	CO ₂ *_s + H*_v <-> COO-H*_s + *_v -> COOH*_s + *_v
R13	COOH*_s + *_s <-> CO-OH*_s + *_s -> CO*_s + OH*_s
R14	H*_t + OH*_s <-> HO-H*_s + *_t -> H ₂ O*_s + *_t
R15	H ₂ O*_s -> H ₂ O_g + *_s
R16	CO*_s -> CO_g + *_s

Table S2. Activation Energies (E_a) and Reaction Energies (E_r) (in eV) of the Elementary Reactions of Methanol Synthesis from CO₂ Hydrogenation.^{1,2}

No.	elementary reaction	E _r (111)	E _a (111)	E _r (110)	E _a (110)
R1	CO ₂ (g) + *_s = bt-CO ₂ *_s	0.28	-	-0.42	
R2 ^a	H ₂ + 2*_s = 2H*_s	0.11	0.98	-0.53	0.22
R3 ^b	H ₂ + 2*_s = 2H*_s	-0.67	0.52	-1.22	0.44

R4	$H^* + CO_2(g) = \text{mono-HCOO}^*$	-0.15	0.18	0.15	0.24
R5	$\text{mono-HCOO}^* = \text{bi-HCOO}^*$	-1.04	-	-1.14	-
R6	$\text{bi-HCOO}^* + H^* = H_2COO^* + ^*$	-0.15	0.64	0.55	1.53
R7	$H_2COO^* + ^* = H_2CO^* + O^*$	0.35	0.42	0.62	0.69
R8	$H_2CO^* + H^* = H_3CO^* + ^*$	-1.17	0.05	-0.43	0.11
R9	$H_3CO^* + H^* = H_3COH^* + ^*$	-0.20	-	-0.04	0.02
R10	$H_3COH^* = CH_3OH(g) + ^*$	0.66	-	0.54	-
R11	$H_2 + O^* + ^* = HO^* + H^*$	-0.40	0.51	-1.16	0.29
R12	$H^* + \text{bt-CO}_2^* = \text{COOH}^* + ^*$	0.70	1.39	0.51	1.26
R13	$\text{COOH}^* + ^* = \text{CO}^* + \text{OH}^*$	-0.39	0.06	0.40	0.79
R14	$H^* + \text{HO}^* = \text{H}_2\text{O}^*$	0.13	0.68	0.16	0.66
R15	$\text{H}_2\text{O}^* = \text{H}_2\text{O}(g) + ^*$	0.44	-	0.88	-
R16	$\text{CO}^* = \text{CO}(g)$	0.08	-	0.10	-

^ahomolytic dissociation and ^bheterolytic dissociation at the O_v site.

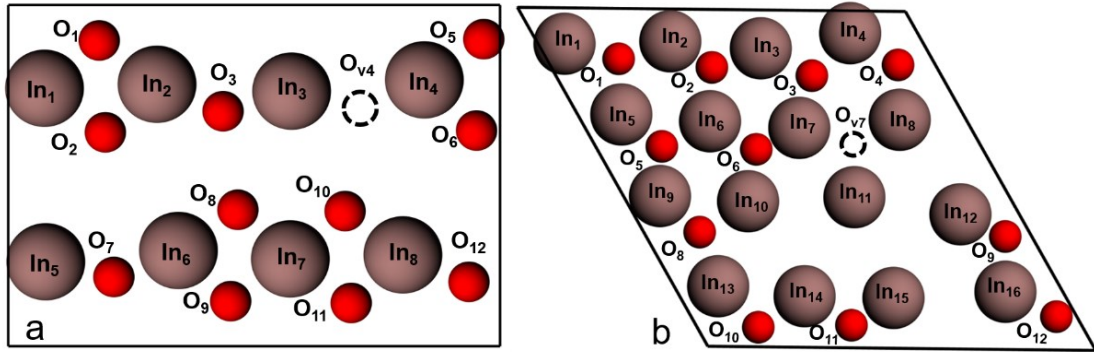


Figure S1. Top views of the defect surfaces: (a) $c\text{-In}_2\text{O}_3(110)$, (b) $c\text{-In}_2\text{O}_3(111)$. Only surface atoms are explicitly shown in (111) and (110), the oxygen vacancy site is shown as black dash line circle. The O and In atoms are shown in red and brown, respectively.

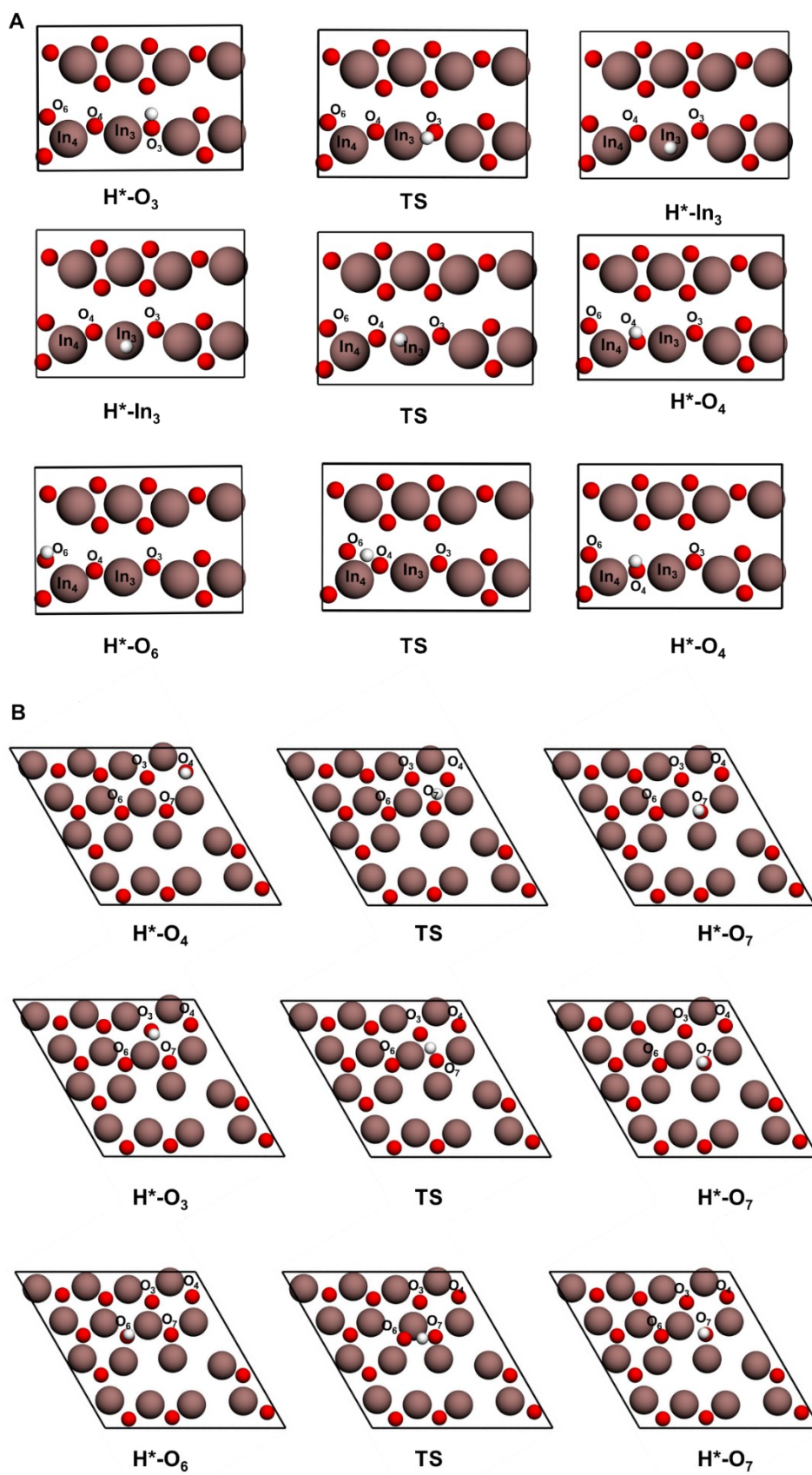


Figure S2. Adsorption structures and transition-state structures of hydroxyl hydrogen migration. (A) $c\text{-In}_2\text{O}_3(110)$, (B) $c\text{-In}_2\text{O}_3(111)$.

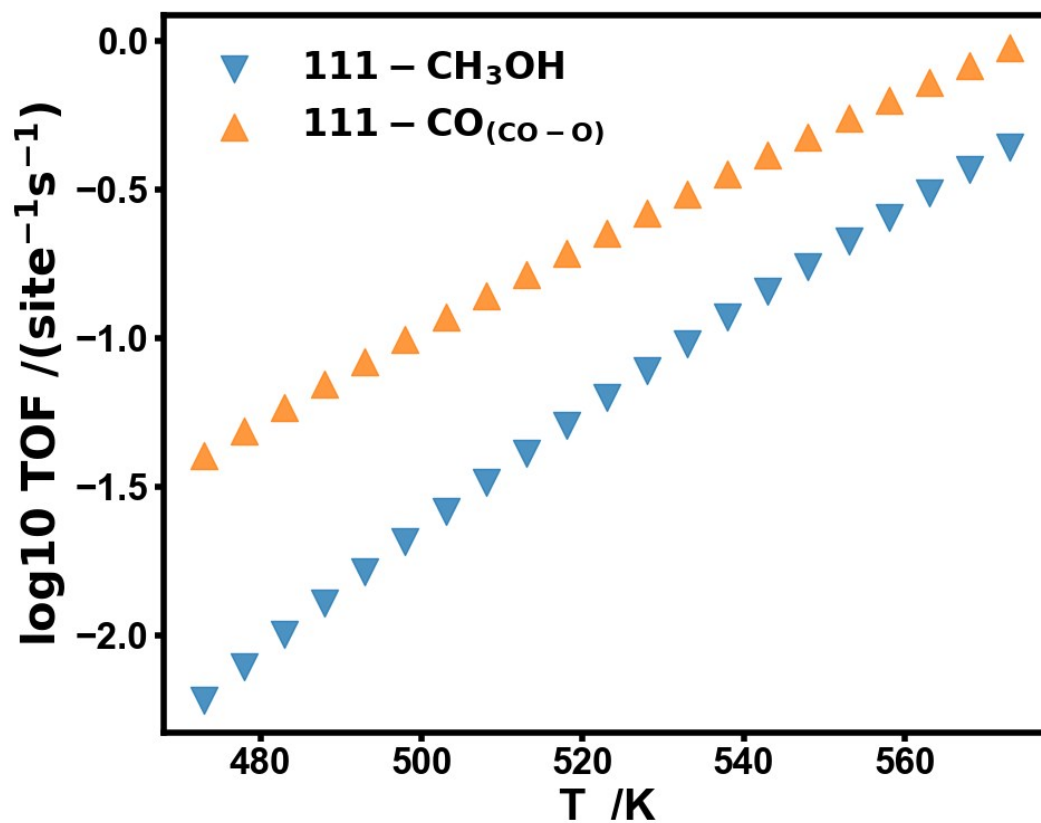


Figure S3. Calculated turnover frequencies (TOFs) of CH₃OH, CO over the active site (the O_V site) of c-In₂O₃ (111) as a function of temperature at P_{total} = 50 bar. Simulation conditions: CO₂ : H₂ : H₂O : CH₃OH : CO = 0.1 : 0.4: 0: 0 : 0.

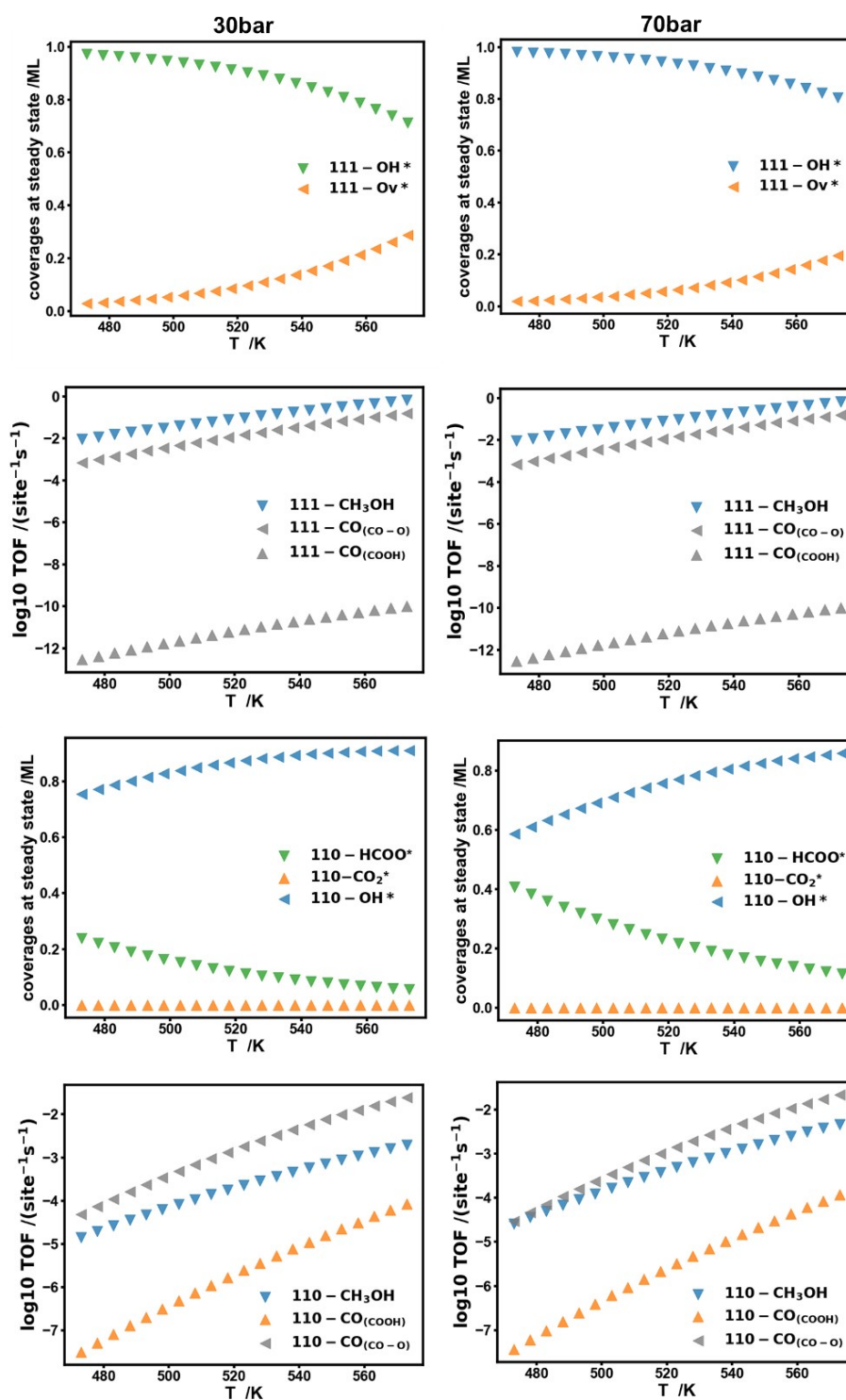


Figure S4. Calculated turnover frequencies (TOFs) of CH_3OH , CO and their surface coverages at the steady state over the active site of $\text{c-In}_2\text{O}_3$ (110), (111) as a function of temperature at $P_{\text{total}} = \{30\text{bar}, 70\text{bar}\}$. Simulation conditions: $\text{CO}_2 : \text{H}_2 : \text{H}_2\text{O} : \text{CH}_3\text{OH} : \text{CO} = 0.1 : 0.4 : 0.0101 : 0.01 : 0.0001$. Colors: gray denotes negative reaction rates.

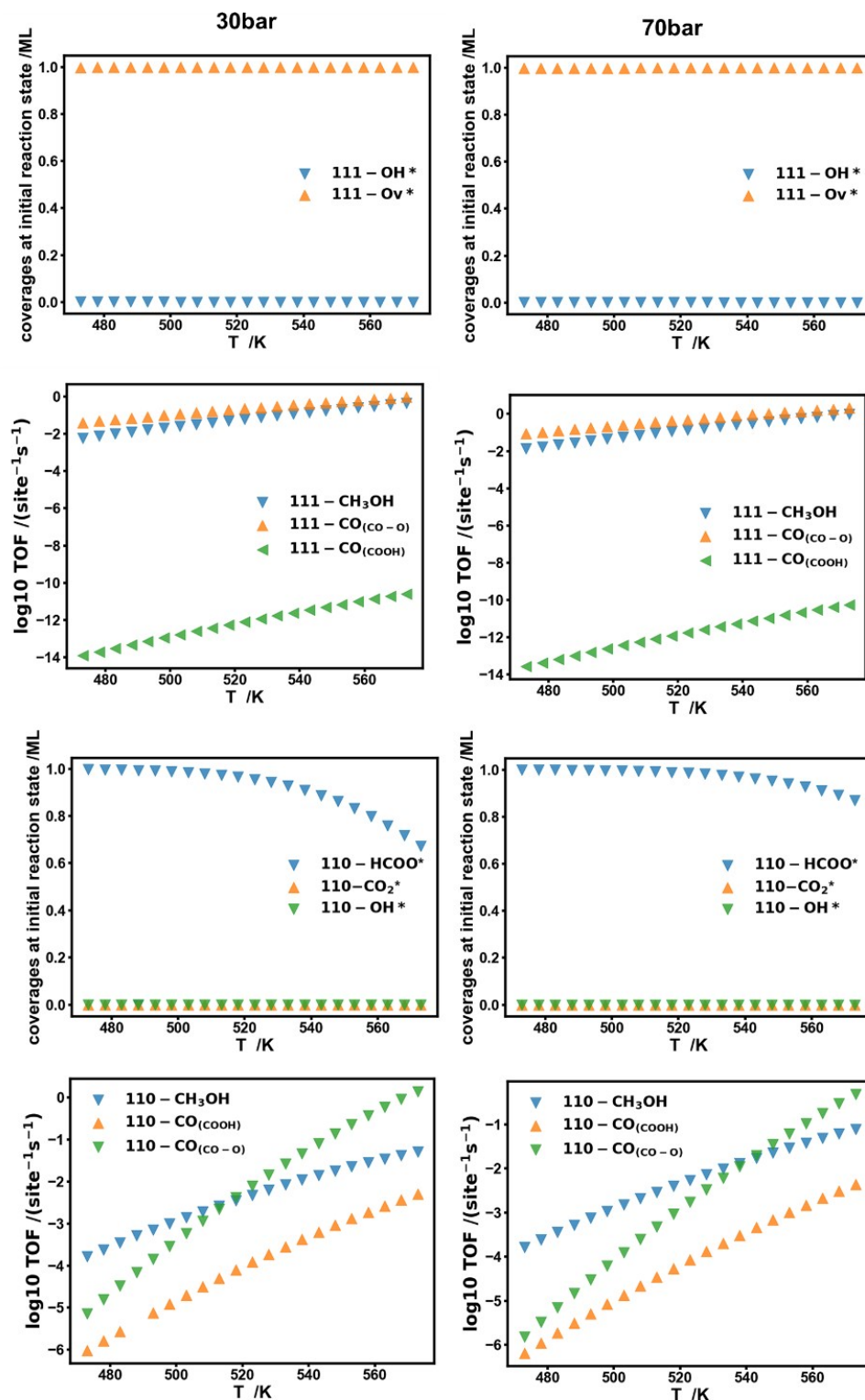


Figure S5. Calculated turnover frequencies (TOFs) of CH_3OH , CO and their surface coverages at the initial reaction state over the active site of $\text{c-In}_2\text{O}_3$ (110), (111) as a function of temperature at $P_{\text{total}} = \{30\text{bar}, 70\text{bar}\}$. Simulation conditions: $\text{CO}_2 : \text{H}_2 : \text{H}_2\text{O} : \text{CH}_3\text{OH} : \text{CO} = 0.1 : 0.4 : 0 : 0 : 0$.

As shown in Figs. S4 and S5, the reaction rates of CO and CH₃OH on the (111) surface do not change as the pressure increases at both the steady state and initial reaction conditions. For the (110) surface, the reaction rate of CO in the CO-O pathway is inhibited by the increasing pressure. However, the formation rate of methanol increases as the pressure increases. These results indicate that increasing the reaction pressure can improve both the CO₂ reaction rate and methanol selectivity, consistent with the experimental observations.³

References

- 1 S. Dang, B. Qin, Y. Yang, H. Wang, J. Cai, Y. Han, S. Li, P. Gao and Y. Sun, *Sci. Adv.*, 2020, **6**, eaaz2060.
- 2 B. Qin and S. Li, *Phys. Chem. Chem. Phys.*, 2020, **22**, 3390-3399.
- 3 O. Martin, A. J. Martin, C. Mondelli, S. Mitchell, T. F. Segawa, R. Hauert, C. Drouilly, D. Curulla-Ferre and J. Perez-Ramirez, *Angew. Chem. Int. Ed.*, 2016, **55**, 6261-6265.

List S1. Optimized fractional coordinates of CO₂ direct dissociation on the (110) and

(111) surfaces of In_2O_3 .

CONTCAR@(110)

O In

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O	In
48	32

Direct

0.6083245259930101	0.1821264671211781	0.4369314914868786
0.1083245259930101	0.6821264671211783	0.4369314914868786
0.1094423919556017	0.9648889494703605	0.4555490458465885
0.6094423919556018	0.4648889494703607	0.4555490458465885
0.3254839097764618	0.5826154986032441	0.3473434527329931
0.8254839097764617	0.0826154986032443	0.3473434527329931
0.8260119012636379	0.5646718411326769	0.5352204026412537
0.3260119012636380	0.0646718411326768	0.5352204026412537
0.1004219979444910	0.9668892360221089	0.6656418364162483
0.6004219979444909	0.4668892360221090	0.6656418364162483
0.3268342710161813	0.8182554151873892	0.3459857086012537
0.8268342710161811	0.3182554151873895	0.3459857086012537
0.6043264108920632	0.6849218489701205	0.6826527891848727
0.1043264108920632	0.1849218489701207	0.6826527891848727
0.8351873760513197	0.3289407270304838	0.5384215215617409
0.3351873760513197	0.8289407270304839	0.5384215215617409
0.5603198096997465	0.6966055874375162	0.4614038208948439
0.0603198096997465	0.1966055874375163	0.4614038208948439
0.3878749774870490	0.0665113626857535	0.3210262989367380
0.8878749774870491	0.5665113626857535	0.3210262989367380
0.8758552271728078	0.0847200035976172	0.5582681874750006
0.3758552271728076	0.5847200035976172	0.5582681874750006
0.0600022524813343	0.4586144971912988	0.4423441288206358
0.5600022524813342	0.9586144971912990	0.4423441288206358
0.7981745481254887	0.2150320941343620	0.6877828275537804
0.2981745481254885	0.7150320941343619	0.6877828275537804
0.3116110813290080	0.4368159706091838	0.6797058336331885
0.8116110813290079	0.9368159706091912	0.6797058336331885
0.0939519125277642	0.3204494196847384	0.3151641112159138
0.5939519125277641	0.8204494196847385	0.3151641112159138
0.6069832052626178	0.8391776284119709	0.5755104970409297
0.1069832052626180	0.3391776284119709	0.5755104970409297
0.3325028680245388	0.4267361666505883	0.4595802297659905

0.8325028680245388	0.9267361666505883	0.4595802297659905
0.0906156151701323	0.0851888438323453	0.3123989733144618
0.5906156151701323	0.5851888438323454	0.3123989733144618
0.8287492314427877	0.7205160016581006	0.4368488425073815
0.3287492314427878	0.2205160016581006	0.4368488425073815
0.5969680260378609	0.0702756450605777	0.5839005657608227
0.0969680260378609	0.5702756450605776	0.5839005657608227
0.8733479963169554	0.6974235394837567	0.6686262633829152
0.3733479963169555	0.1974235394837567	0.6686262633829152
0.0299855786212778	0.8338910272029311	0.3248344274949237
0.5299855786212778	0.3338910272029309	0.3248344274949237
0.5577861535883214	0.3121980128475415	0.5629086586615525
0.0577861535883213	0.8121980128475415	0.5629086586615525
0.3681071436100752	0.9523566886389767	0.6848389463557006
0.8681071436100753	0.4523566886389767	0.6848389463557006
0.9672759671817451	0.2175983719279826	0.5835172190098384
0.4578538593566647	0.9300033519987845	0.3307363800026345
0.9578538593566648	0.4300033519987846	0.3307363800026345
0.4672759671817451	0.7175983719279825	0.5835172190098384
0.2197324264949282	0.5582622499403124	0.4603242710595687
0.2135913345090259	0.0915199140799826	0.4218602716772820
0.7135913345090260	0.5915199140799826	0.4218602716772820
0.7197324264949282	0.0582622499403124	0.4603242710595687
0.7442686059226477	0.5736682497383089	0.6646180386591415
0.1810906058802965	0.8248172259716080	0.4406759257175549
0.6810906058803037	0.3248172259716079	0.4406759257175549
0.2442686059226478	0.0736682497383088	0.6646180386591415
0.4637282660104010	0.1825048902876900	0.5476389979558557
0.9665882210905902	0.9710311937642538	0.3526635163161322
0.4665882210905903	0.4710311937642537	0.3526635163161322
0.9637282660104008	0.6825048902876899	0.5476389979558557
0.2199054115163663	0.8461698077476828	0.6541673871320134
0.2326256230663724	0.3025488623554788	0.6742497598409138
0.7326256230663721	0.8025488623554788	0.6742497598409138
0.7199054115163662	0.3461698077476826	0.6541673871320134
0.6775389983872484	0.8257319870091754	0.4430542472349913
0.2531828865435875	0.5763537505404928	0.6678055386742539
0.7531828865435876	0.0763537505404925	0.6678055386742539
0.1775389983872482	0.3257319870091754	0.4430542472349913
0.9609977302614578	0.1997461439757086	0.3405149960056238
0.4648266290139202	0.9512583181384436	0.5655751466348635
0.9665031589122641	0.6993840020164299	0.3396446202806125
0.4659718640619485	0.4474392078428522	0.5667648225121296
0.9659718640619485	0.9474392078428522	0.5667648225121296

0.4609977302614580	0.6997461439757086	0.3405149960056238
0.9648266290139201	0.4512583181384435	0.5655751466348635
0.4665031589122640	0.1993840020164299	0.3396446202806125

CONTCAR@(111)

O In

1.0000000000000000		
14.4443000000000001	0.0000000000000000	0.0000000000000000
-7.2221499999999995	12.5091307398835685	0.0000000000000000
0.0000000000000009	0.0000000000000016	15.0371000000000006

O	In
48	32

Direct

0.1440391158916853	0.8159113304919428	0.3527222041353459
0.4677202504530226	0.4773858667252213	0.5383266426614446
0.7700602015015957	0.4904786959724184	0.5699651659636774
0.4256005208406664	0.8266999416362480	0.3506182360926144
0.2892543147220137	0.2738231848488950	0.6220510764572736
0.9312002251200319	0.5968025569714553	0.3606023751194078
0.4845842717073146	0.7443525371612074	0.5250367150051848
0.1599693366589443	0.0699891093784374	0.3209629232473715
0.1825844287610761	0.3322071127980764	0.3453041630151077
0.5227075956461518	0.9907938533551851	0.5398847327568513
0.5098971966419437	0.2794979080171272	0.5699695103183593
0.1729186823798735	0.6019194383870307	0.3534190685579894
0.7292760845930455	0.0162449661013302	0.6293723631694463
0.4038973912880883	0.3366719810481560	0.3548820415870771
0.2592210305128240	0.7464601586794584	0.5251102439721942
0.9332649532345049	0.0924248097684213	0.3252217730935224
0.6682379524415855	0.8536960816015965	0.3445170733949186
0.0072448935580858	0.5281346055230918	0.5407453556221654
0.7188679173052900	0.2299019514514861	0.5703282536565940
0.3970486975002454	0.5739336893753630	0.3508024603853359
0.9886883188259461	0.7201300392879481	0.5675541226420160
0.6641298630934108	0.0677650978431490	0.3574002804196527
0.2567482429909881	0.5156329745511721	0.5256767740965703
0.9112235864764573	0.8417912596938969	0.3309222157076874
0.1871524123849016	0.8505994667901696	0.6429173961455045
0.8548202303834292	0.1734662474223119	0.4590897502024882
0.5595323597405512	0.1735382685120809	0.4221269427654583
0.9029844151633810	0.8421911674841872	0.6397043934887058
0.0526691042126740	0.3952914258770677	0.4309689926683100
0.4017485672560586	0.0681952382108443	0.6338352991837191

0.8401672201574860	0.9338645770941177	0.4693946533791372
0.1720130491447631	0.5928671442685994	0.6658518500821226
0.1451847970866641	0.3381502299830350	0.6372132077206840
0.8125390294142207	0.6752856735417930	0.4527416433614847
0.8247910742699386	0.3846933302433830	0.4221688564018395
0.1574938738230078	0.0578599779496756	0.6390089664558597
0.6014896773273717	0.6591793194386378	0.4289852062209413
0.9297418252052592	0.3329820937836050	0.6355883945998793
0.0713635600906908	0.9212087958965385	0.4678595035427559
0.4106465346790476	0.5841713539899362	0.6669243820468657
0.6636280789836375	0.8075605111639041	0.6336078064435223
0.3192108417469892	0.1466548508879880	0.4562044460969578
0.6119195798995763	0.4381113055830360	0.4221517910996896
0.9463757217834357	0.0982657007864254	0.6366202069057016
0.3418414963077996	0.9488823879894898	0.4293892782685255
0.0935271749667575	0.1598962692176550	0.4676375869858496
0.4176430198237965	0.8276947904785645	0.6688154856560102
0.6661702718348245	0.5974028319655575	0.6325524855137843
0.1124930286148554	0.6849606917684345	0.6041213289382990
0.5518058541790625	0.1507770526512085	0.5730901611511112
0.2299641200935606	0.4925796927067300	0.3860820387527369
0.7776197762994794	0.0149762809391053	0.3827531081268519
0.3156834853495620	0.4303629768325539	0.6120949303159224
0.8464565904927188	0.3991269303229203	0.5736412516713071
0.5067211716085982	0.7403484117866946	0.3852096882999290
0.9843833337124562	0.7616415320773406	0.4003373897693630
0.5719149624358481	0.8876250997840583	0.6127525104677716
0.5981028593878196	0.4471085526306647	0.5729154774356769
0.2598660541712691	0.7706681081260367	0.3853488156381541
0.2373272484215436	0.2243004517201335	0.3795757630066327
0.2197745324485126	0.9835462685363593	0.3931454061539787
0.7803386784395785	0.5133910154945186	0.4212470264149660
0.1124998867101695	0.1779302433713255	0.6125694139937473
0.5561169753984216	0.6520354691863114	0.5879413554597669
0.0192263783229016	0.2387029979330212	0.3975663992406723
0.4832511446369852	0.2667276282542175	0.4219969195974634
0.8246617444763610	0.9332613603339311	0.6139705026795382
0.3463816627730495	0.9042681825392854	0.5941267555250301
0.7602622689917308	0.7824322963662208	0.3940656538125241
0.7327585521882649	0.2160144363765059	0.4237460572388410
0.0690999916624623	0.8940868011954063	0.6089744875580911
0.0945595153197094	0.4436620795085353	0.5919960110186236
0.0103841090732853	0.5134786209649856	0.3984448999870493
0.0010738950756379	0.0016701224883896	0.3866558672282420

0.4839958727272949	0.4985492124419224	0.3966833341531972
0.5012249012285330	0.9882202473741728	0.3982857917723686
0.8282862033124335	0.6794538804805846	0.5958383462739222
0.3226279726062559	0.1524934282889397	0.6022319292611260
0.3334018620327271	0.6677215759974103	0.6094691880090848
0.8505409155922211	0.1698252739732346	0.6054483391627665

CONTCAR@bt-CO₂(110)

O In C O

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O	In	C	O
47	32	1	2

Direct

0.6088491824254844	0.1834521406383011	0.4332802317445461
0.1083493378634993	0.6841293483540193	0.4392189777377315
0.1101414083524843	0.9654781530188505	0.4544497886803130
0.6097994722442340	0.4671316624657623	0.4549086939070485
0.3249167509784570	0.5857103468411570	0.3517601098727444
0.8269886280776312	0.0835419357763800	0.3446581470222118
0.8270389557970422	0.5662620409377828	0.5335882898610976
0.3285813601220333	0.0646472758160601	0.5306585173587994
0.0949405352082040	0.9785751366379630	0.6620596284546053
0.6032011955451296	0.4682303386033919	0.6651801618017219
0.3283536235807855	0.8202827441475627	0.3490111427506239
0.8274019754639219	0.3197910601249125	0.3440797716416731
0.6023068889689753	0.6872335904672587	0.6817294019421216
0.1024585131371769	0.1861749774937187	0.6816076889632812
0.8356612624965633	0.3299817773830721	0.5358774820173590
0.3346991252909506	0.8254338845182256	0.5444753451120671
0.5616527338767773	0.6961505835177030	0.4585678694002827
0.0616011513962460	0.1971510263233375	0.4594183138766808
0.3888397058648158	0.0683296839380877	0.3181195447111524
0.8890218180854829	0.5679096368810952	0.3201874713338277
0.8742578124949353	0.0869392213362565	0.5551195544586701
0.3703690350945785	0.5873641362458548	0.5710214802439413
0.0622402470709246	0.4602708940864190	0.4401582815303072
0.5606901034230363	0.9590589311583196	0.4401206313320007
0.7995703197262740	0.2161211955972861	0.6860975871142645
0.3233642181789950	0.4241449276390780	0.6761454113962482
0.8108188976068601	0.9382409240233185	0.6766096582332064

0.0950123335358711	0.3212116402808088	0.3137809258610795
0.5929491839378985	0.8214129390296740	0.3127360135163226
0.6089025756216854	0.8396288742361773	0.5722454182909041
0.1065792657215826	0.3396497919044860	0.5732989202648666
0.3336706046638789	0.4296803336359265	0.4615399068869604
0.8328299479412664	0.9281592717921630	0.4562880524215509
0.0918022947504460	0.0859010960276928	0.3104204934094461
0.5893411002749558	0.5861484826972430	0.3104787166582859
0.8293792480075519	0.7217107512241343	0.4357081718343618
0.3292899386064491	0.2224814531574844	0.4344620717869851
0.5984598744636127	0.0711692588350220	0.5807992477801996
0.0994903734050472	0.5681421876156834	0.5842713791352745
0.8715488441527702	0.6982323831056457	0.6669929192865739
0.3759607685271052	0.1967465831548396	0.6642803888825395
0.0319605448579811	0.8344806545276189	0.3241984121243442
0.5284994666973410	0.3367698175626170	0.3239818928545445
0.5610275455873829	0.3130776286807540	0.5606186222538073
0.0577282334417295	0.8152001258930499	0.5655401560032346
0.3692486338513380	0.9598337992325894	0.6822581445245675
0.8702400942626703	0.4528705965538087	0.6826501188267375
0.9670475633988332	0.2188606953896232	0.5808376689668684
0.4579375027818946	0.9318806288089662	0.3286461469206179
0.9594424273453545	0.4311320615624629	0.3291907740807943
0.4739611092598377	0.7158955925889295	0.5786892980140740
0.2211880241057021	0.5604053309985358	0.4659804869678602
0.2146092879891565	0.0926812411361709	0.4193163882693815
0.7161016523590206	0.5919318750080718	0.4190043016507419
0.7199281130435961	0.0597934888695404	0.4571774780642122
0.7458304546395220	0.5745902460243236	0.6636486928141799
0.1817841965334201	0.8257898993587156	0.4423805229468818
0.6811377035954330	0.3267500997503726	0.4386288656877465
0.2463170877058331	0.0788739265040320	0.6601972058997168
0.4661766020396297	0.1836900822353738	0.5438172606826017
0.9684341824072594	0.9717775489002622	0.3502569460378271
0.4651403863085208	0.4734645748266803	0.3532983781889823
0.9664001040179556	0.6828022141228741	0.5483166614068661
0.2152542304552424	0.8619504580679258	0.6542840558735985
0.2316979175999751	0.2988809757424646	0.6718173336149638
0.7325102841014420	0.8040223992520903	0.6729185204234858
0.7218474328169752	0.3472538281748521	0.6525782246277780
0.6791534533966503	0.8266911626169082	0.4398227665746689
0.2435645260122244	0.5559097497213469	0.6810036381468465
0.7533679260008809	0.0781991132807378	0.6655957554697983
0.1785889283644962	0.3276034508661599	0.4418872036862327

0.9618602234313108	0.2009713736408802	0.3387986273576391
0.4673691882009722	0.9520668446073580	0.5637500669435143
0.9687875191101749	0.7002855672869122	0.3396175576988856
0.4673538244226190	0.4481118093221138	0.5676730722080477
0.9628738816375890	0.9497829292815854	0.5636282829132209
0.4606123732106001	0.7010232085198222	0.3387147802586589
0.9643920393678391	0.4519734909323367	0.5625386523148806
0.4662124745197181	0.2016946402899377	0.3366093612017377
0.2198567211488879	0.6825133039933038	0.7579724496764664
0.1497557786124658	0.6992096838399794	0.8170258783676223
0.2876397493789152	0.7405212613597384	0.7107875409414657

CONTCAR@TS-CO-O(110)

O	In	C	O
1.0000000000000000			
10.2136999999999993	0.0000000000000000	0.0000000000000000	
0.0000000000000009	14.4443000000000001	0.0000000000000000	
0.0000000000000010	0.0000000000000010	15.9874000000000009	

O	In	C	O
47	32	1	2

Direct

0.6087160353988402	0.1828343750890691	0.4352372964911980
0.1081106298941842	0.6827825324584537	0.4359427760857905
0.1106007819117442	0.9652360909664042	0.4541433969704669
0.6090837444216832	0.4662243667570508	0.4548240107890187
0.3253992215776467	0.5841369126068129	0.3481753803587236
0.8259251511233878	0.0832295524105521	0.3459463584577249
0.8262728103896186	0.5656663528242346	0.5332363568051777
0.3276507138644252	0.0644273874474170	0.5327151933779716
0.1010210329507577	0.9682990430480071	0.6638802638915148
0.6014263618979439	0.4678069368983045	0.6648210095033427
0.3274343128223896	0.8193153680487367	0.3464092716558096
0.8265756145920538	0.3191548382474551	0.3444248385890493
0.6023443478562507	0.6865659356522301	0.6812823302560675
0.1052765451855943	0.1849553710088556	0.6810418692663387
0.8352715156943809	0.3293168319990211	0.5365756164797374
0.3357432080414464	0.8260243725105405	0.5401217153655160
0.5617031943445976	0.6966226801243922	0.4585482504899248
0.0606517458606500	0.1969771407197883	0.4599520143361089
0.3881598665776599	0.0676600612134832	0.3190445773290529
0.8885329205934575	0.5671687906307921	0.3190546405846291
0.8765306779519451	0.0851197117839050	0.5569538750480262

0.3736894669756767	0.5873106746014152	0.5626442008552007
0.0604654942769539	0.4593245894093857	0.4405144300548093
0.5604119338105683	0.9588748536181786	0.4405878772026134
0.7990311704070709	0.2156350178320432	0.6862091064091375
0.3139769257218894	0.4340418233425583	0.6759434453562841
0.8121580500938387	0.9374665679568801	0.6788911506647968
0.0941929580551898	0.3208707794759659	0.3139091762712282
0.5933846054670110	0.8213648754131591	0.3127738744341119
0.6094653652118848	0.8395987244332965	0.5726191476856647
0.1064912960385028	0.3393286968698629	0.5739705986834287
0.3323822232478180	0.4286163159220193	0.4599501980913883
0.8333476926838829	0.9275718733764013	0.4577858619470500
0.0909315346072069	0.0859089462399195	0.3109781019151477
0.5898956771518526	0.5855740372308810	0.3102454477070396
0.8289249067642872	0.7209988791169253	0.4344203063333406
0.3288666327173620	0.2215308495291475	0.4355865919788645
0.5982293738521133	0.0702560035376846	0.5820372281911724
0.0969450548586064	0.5702235918857369	0.5823287977147376
0.8720923754911082	0.6977929535213908	0.6671015853216328
0.3748103989415049	0.1966491989208589	0.6665402079063298
0.0304167972285897	0.8345940451103597	0.3232093782631851
0.5288746691916264	0.3352968853241902	0.3241409770321472
0.5584145334660575	0.3129260248679321	0.5616168321069203
0.0575733074711663	0.8130806198699383	0.5615335484839780
0.3694660824470434	0.9534517926595785	0.6830304888485805
0.8689053559553006	0.4531105346819193	0.6827949881478779
0.9678041050956718	0.2180416589217587	0.5821130253958197
0.4576496120876480	0.9311999258504531	0.3291246815859417
0.9582440912400554	0.4305233190182058	0.3290598682691741
0.4719593949416117	0.7174755117002253	0.5794129879234586
0.2196251762527822	0.5594360992452074	0.4612369283894944
0.2140655090944639	0.0922659878773708	0.4202551029513830
0.7148464739608898	0.5915967808964900	0.4190532314611138
0.7202426067378035	0.0588812755559718	0.4589285701672968
0.7443305217412701	0.5743850818558603	0.6626268336164108
0.1813580715703304	0.8250231233287590	0.4406371226387977
0.6806809865743318	0.3260437142199750	0.4393115500843218
0.2458763261376486	0.0741404916680057	0.6623993676140925
0.4650787273209164	0.1827419264045227	0.5458144659122766
0.9675240837783499	0.9716617795559731	0.3511321671517720
0.4658627488828340	0.4722742497837904	0.3524875747805316
0.9638480446462390	0.6832367268968377	0.5462127122719073
0.2194197397053594	0.8475215179984160	0.6553124306482534
0.2337627693083132	0.3015685264900463	0.6721021871256665

0.7326489942121349	0.8036887295188984	0.6729400934494542
0.7206882257725491	0.3468578591545900	0.6525213679461097
0.6791142313001926	0.8266099983787721	0.4400810154430893
0.2473215777915662	0.5733046405589175	0.6706557067383538
0.7537720860352081	0.0769827795712257	0.6664288129347526
0.1777357779463011	0.3266153245303746	0.4419726714692726
0.9609599406020609	0.2004918949468227	0.3393402771277395
0.4657387776683184	0.9510564612950710	0.5641018479041132
0.9675773914290146	0.7000481277820644	0.3378116024565649
0.4644937386801171	0.4477575630479212	0.5675700408612688
0.9667689300917580	0.9481736963811407	0.5651526842273581
0.4609923596228399	0.7006109296086469	0.3384631713312802
0.9645315490563808	0.4515630571797321	0.5633441529202757
0.4664575975372808	0.2004598951279526	0.3381850928208461
0.2094864651758405	0.6375641288314708	0.8035900379302614
0.1808980573052620	0.6799387136769894	0.8618909305034885
0.2757740762174331	0.7171298800515068	0.6994014682444588

CONTCAR@CO(110)

O In C O

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O	In	C	O
47	32	1	2

Direct

0.6093023284901843	0.1834106709809935	0.4345855718812257
0.1088013688062425	0.6831008629375124	0.4369423291646745
0.1100054366017666	0.9659676684969313	0.4543932307240429
0.6097575212485581	0.4663334872885334	0.4554693118003139
0.3252472363786992	0.5842787565320862	0.3487598019925477
0.8263170137278563	0.0832999808013222	0.3455041674981892
0.8263463009044529	0.5656628985816067	0.5343395697670542
0.3267997458640497	0.0646387652193269	0.5327837166104653
0.1007846067230793	0.9669831660495990	0.6647566460910972
0.6018797024258907	0.4671805322112600	0.6658203054421398
0.3273711687247461	0.8200922632446366	0.3471244154727312
0.8272141863166865	0.3197422047151047	0.3443104371945395
0.6045548534345300	0.6862755870764443	0.6823702145361686
0.1061361878612680	0.1851600072118389	0.6803510897316049
0.8364762429816904	0.3298164668512498	0.5367130492105511
0.3347681119024359	0.8279465536149858	0.5393531480973306

0.5609573475821223	0.6977240919273985	0.4608695072192759
0.0613046335776670	0.1976120825696816	0.4593933666458459
0.3890553507943642	0.0681900153174846	0.3182940441055468
0.8888527915487315	0.5678899613291113	0.3196814849047946
0.8768659121493874	0.0855690337168281	0.5564918207123568
0.3753495609926703	0.5864081712457817	0.5610488340869930
0.0610283450648241	0.4599790529679492	0.4413276656385006
0.5600037344652116	0.9592323815928757	0.4410726610042842
0.7996380073895228	0.2157333094680316	0.6862919368595791
0.3111720101651167	0.4370998968675444	0.6780698476663437
0.8122857921723015	0.9380233176409287	0.6782374569721310
0.0947124996628907	0.3220008630313632	0.3137925197166831
0.5933367944861568	0.8215326677973229	0.3137343253316804
0.6080671029237693	0.8400556668809328	0.5743026055820027
0.1075764187952285	0.3398386918410416	0.5738533139313379
0.3329185847497835	0.4281344444057993	0.4607034136603349
0.8329564798506585	0.9277548760588560	0.4578825876271239
0.0911410832936224	0.0861527408682018	0.3104932742538429
0.5897869396197747	0.5868080019588395	0.3118067041491435
0.8289193250938184	0.7214132550123495	0.4357162238499679
0.3293648754733537	0.2214182095907211	0.4346951067112550
0.5975166804148739	0.0707351270310968	0.5815453652803105
0.0972161686619856	0.5715549830857005	0.5834745029212247
0.8735384005308255	0.6980362785797303	0.6686318186420227
0.3743440603619422	0.1975178825387190	0.6656345500619820
0.0311119690051516	0.8347449719977940	0.3239055877112767
0.5290613019816923	0.3362538544315538	0.3236434136021435
0.5586311091955433	0.3131249639199307	0.5617036576772357
0.0565724984791113	0.8131176807927891	0.5619412595952805
0.3686836283266423	0.9529335835314390	0.6836394108259005
0.8697496091556364	0.4534515560511903	0.6837010470817353
0.9688093877144084	0.2181994147962422	0.5816744151469876
0.4579947422197115	0.9315464462504124	0.3293816514847862
0.9587354165659906	0.4315660277809122	0.3297602143262308
0.4682625129342178	0.7183738002978002	0.5832762427703824
0.2203649853274670	0.5596455054369123	0.4619994193239627
0.2144189676972005	0.0924162452918572	0.4196719066902552
0.7139472892513270	0.5926268196298297	0.4207298111240773
0.7201003037056619	0.0589892190045120	0.4584245805706800
0.7444275136476496	0.5745110553595303	0.6634841474449467
0.1811379148829325	0.8256862492379905	0.4411652567623649
0.6814365689051909	0.3265267333661287	0.4393539437494188
0.2453246516133423	0.0736471718800682	0.6623900501197633
0.4645974305413551	0.1830607608374209	0.5450156415205077

0.9676455070663531	0.9717943012593931	0.3512445472505377
0.4662090230968658	0.4729277327846633	0.3534350215854682
0.9631815568333753	0.6833803063319398	0.5469361713671299
0.2192552299428892	0.8459507934498113	0.6549717364263010
0.2344759379074032	0.3028088865137541	0.6718069291023013
0.7333868636524075	0.8037950973133795	0.6732937514190941
0.7215387454825156	0.3467585685624089	0.6523378756464842
0.6780679075880189	0.8268024902667732	0.4415594750221312
0.2494138071644610	0.5782967922191053	0.6703456406670280
0.7532935144163194	0.0774249430674296	0.6655996267020455
0.1784639465538354	0.3269732405907513	0.4416678797164690
0.9613781070501433	0.2009474728355642	0.3389653953410970
0.4646594947952805	0.9512443080697355	0.5643765724172713
0.9680556740381597	0.7003137958278731	0.3392164969086248
0.4645253810131824	0.4480591045837003	0.5686255405277438
0.9664872736368968	0.9484192562472986	0.5655083031062378
0.4603911891393449	0.7013594764465232	0.3406035828968099
0.9659193141235844	0.4522074398845467	0.5643598415661146
0.4672036053723848	0.2012111442817016	0.3373789646477681
0.1842426752035621	0.5614645897500938	0.8266156019160017
0.1641507050390746	0.5576988987296116	0.8966628461112971
0.2938577588837227	0.7169360901838497	0.6924914364556412

CONTCAR@bt-CO2(111)

O In O C

1.0000000000000000

14.4443000000000001 0.0000000000000000 0.0000000000000000

-7.22214999999999965 12.5091307398835685 0.0000000000000000

0.00000000000000009 0.0000000000000016 15.0371000000000006

O In O C

47 32 2 1

Direct

0.1395895154519268	0.8136892506533671	0.3547378989578685
0.4746871007268100	0.4869167126784688	0.5436193656789613
0.7752374252683963	0.4976942682316172	0.5729575988862011
0.4278157426141524	0.8257946936604781	0.3484455950717565
0.2878561306069723	0.2780952275568053	0.5950080449763958
0.9270170500520705	0.5986750951417655	0.3646905376355341
0.4810747534465857	0.7489885195597891	0.5227160792551496
0.1575536687578481	0.0742557040568251	0.3192168923384144
0.1830352347341032	0.3343118895698041	0.3477577335090665
0.5152490013433558	0.9874174474324627	0.5380110619910334
0.5045058643188262	0.2740785876113437	0.5686896645737060
0.1741775321692283	0.6062447991980748	0.3572867283411733

0.7291115720248862	0.0129828575055676	0.6281675910204635
0.4037442489214185	0.3374046325079397	0.3573135258252931
0.2649830168521943	0.7599673578389529	0.5271756300082084
0.9328867306525175	0.0944432000621907	0.3237748603480117
0.6696935234970642	0.8544086225149503	0.3456886862252371
0.0088827655365663	0.5311177131073467	0.5430034319773853
0.7186307824778692	0.2292544960232316	0.5718070890656016
0.3977558899647526	0.5729573490987105	0.3536721966175255
0.9988302702437737	0.7288785693757868	0.5615304739394549
0.6659650869066857	0.0704973856861702	0.3565171368187643
0.2557593430814689	0.5179203293500549	0.5271048818754481
0.9101457402834024	0.8403092463113288	0.3361419152703268
0.1871070077128769	0.8523027040513127	0.6529127861449326
0.8548302131485730	0.1749722693565061	0.4592534703426570
0.5626281550550165	0.1763635683365695	0.4226024286341110
0.9099572437583899	0.8471637485490118	0.6394621314906613
0.0520365051398666	0.3980082603363279	0.4310815336347016
0.4014956026808281	0.0691639514188306	0.6361671373880567
0.8415950211393918	0.9380966540427654	0.4698898317115178
0.1732608046039001	0.5967671982985934	0.6664651506227910
0.1464216622807229	0.3414224438428179	0.6435591279378258
0.8078406102733131	0.6771110491886126	0.4652336899593227
0.8245657400103884	0.3873688599651049	0.4255771665389683
0.1620528585839917	0.0660470592660667	0.6433247221952114
0.6004773579716565	0.6611751925614155	0.4314233588934553
0.9295752000601581	0.3336846213808638	0.6359753052089783
0.0764806184866003	0.9286095383024617	0.4684898292501853
0.4092211642104668	0.5883042580115040	0.6670397941211574
0.6646826016222831	0.8014553458649183	0.6275661686717412
0.3190336089108606	0.1434222775750751	0.4531637655187357
0.6096055579880854	0.4390090330871271	0.4299451395698105
0.9459001568024836	0.1002104723954864	0.6377776136376204
0.3457604782161252	0.9551756321323013	0.3947691337797166
0.0893678763871009	0.1600963851057415	0.4674568281316822
0.4226619033471446	0.8284452916545301	0.6755685308523552
0.1158759482115767	0.6894786864782545	0.6040376879929282
0.5505905954360213	0.1490256241455999	0.5717128530608749
0.2298506386022782	0.4946814554963037	0.3871306765682597
0.7780953403071138	0.0168947769974017	0.3812309447108139
0.3150845888186815	0.4335378499555357	0.6131125191064216
0.8470488786509817	0.4012938205089910	0.5754796739999370
0.5066198776567670	0.7409326822558974	0.3816825236163747
0.9849723599510263	0.7636971635863314	0.4066634563540362
0.5725264635405798	0.8888983171854665	0.6103711075101340

0.5934688331895288	0.4410397387763754	0.5875981937204848
0.2629640973802392	0.7770062461652817	0.3838096360525652
0.2371626564371581	0.2259044738091002	0.3843789291972780
0.2186148929556928	0.9850493954997182	0.3837752280802891
0.7774595415707140	0.5157863456245995	0.4267063180087630
0.1119027053151782	0.1816620832339796	0.6107064162921689
0.5462726679983994	0.6552787071465882	0.5797742464728759
0.0185474387709400	0.2411914585095647	0.3960767848198487
0.4835789591271150	0.2666690134298216	0.4216065172554772
0.8276567293578602	0.9337405373838212	0.6135255914529664
0.3480250508436473	0.9053156038813932	0.6113896485252003
0.7607609733453339	0.7845869145705315	0.3998811349657188
0.7340434653535889	0.2188547509158203	0.4240258231341377
0.0766370275194107	0.9029141108493079	0.6093862863143791
0.0942065686087050	0.4451588752893253	0.5937717908030966
0.0103198522945020	0.5178136218923562	0.4003567576212817
0.0009165862696934	0.0037224747890894	0.3867168811726393
0.4857891877415120	0.4979618043499482	0.3998970983500227
0.5026442870459120	0.9894872919758820	0.3932413232723245
0.8423347762858698	0.6817047110840547	0.6037968366509696
0.3237847474931598	0.1550823902336702	0.5983103985764784
0.3320112515578862	0.6709647863368332	0.6104957253272345
0.8488694013807307	0.1699284069988506	0.6050254844314950
0.5863473367104310	0.4986371926763813	0.7812336973222258
0.7434951081463006	0.6212318231326112	0.7192671592990753
0.6488052278023761	0.5374370953783650	0.7196053855180257

CONTCAR@TS-CO-O(111)

O In C

1.0000000000000000

14.4443000000000001 0.0000000000000000 0.0000000000000000

-7.2221500000000001 12.5091300000000007 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0371000000000006

O In C

49 32 1

Direct

0.1375864475351665	0.8114021886430365	0.3571481112373538
0.4747741782305538	0.4829289900200161	0.5461080011330547
0.7677299206965178	0.4928790937605219	0.5743969015081181
0.4280126244930791	0.8227421948404398	0.3522677820722808
0.2870173869442948	0.2762264272097075	0.6036547520548011
0.9268895790055243	0.5967717148247235	0.3633702018712152
0.4826188853590797	0.7448987381407235	0.5274767710952697
0.1561441701705893	0.0731574155065825	0.3188677035264224

0.1818921531974612	0.3335819754219599	0.3469078985450336
0.5101776035992401	0.9850222849198604	0.5369052782944365
0.5017120797947410	0.2704911112918451	0.5675267073442979
0.1743786210034504	0.6055782571265871	0.3568539065362710
0.7271486777014045	0.0183185790646462	0.6226171390210967
0.4025012444827628	0.3370585241511940	0.3592928447820895
0.2637705486137510	0.7607336497331939	0.5261502231551155
0.9318265103010698	0.0937534299305904	0.3250296576807776
0.6685552204253143	0.8539878803080566	0.3470058697323157
0.0062976334151980	0.5308213630491402	0.5423391314175376
0.7162753585936947	0.2295568542050302	0.5716040814898002
0.3982851873343449	0.5715402469149278	0.3553739663973765
0.9917483343538249	0.7257388619149514	0.5652762343782052
0.6651818750491036	0.0693710049876735	0.3578923869502927
0.2564727862525015	0.5174099067864704	0.5268713196184244
0.9102747013518686	0.8419789412657364	0.3339148216166577
0.1836397017811493	0.8500838477390913	0.6525653704568402
0.8552881255576871	0.1769376860563390	0.4588752464300513
0.5607882752112485	0.1748009066023873	0.4218792347874957
0.9068603430666924	0.8485262921685826	0.6409046764933901
0.0522033408598506	0.3982617479496774	0.4313070980709905
0.3988719065509030	0.0670827149477134	0.6365618572488630
0.8410918551005914	0.9366827483258826	0.4707146337709674
0.1733903550170785	0.5970669054175435	0.6641407967363112
0.1452610789941637	0.3413816068973030	0.6414215726553523
0.8101368909410435	0.6766785468386191	0.4580088497824166
0.8230317000173341	0.3864537753097499	0.4257492363363307
0.1587976378106709	0.0632535106697493	0.6425513972432821
0.6021324438963734	0.6608912886360980	0.4351970262532502
0.9288783936625714	0.3356695340794992	0.6363383786156868
0.0744122002734961	0.9265249982689914	0.4683744241294449
0.4099586085650769	0.5859758775947369	0.6689343086127341
0.6638135560701034	0.8106007715544558	0.6339702879283712
0.3165700408916625	0.1409902305087773	0.4533886042439051
0.6092325822459126	0.4371898782059921	0.4286015229788570
0.9448332181157487	0.1016368259724618	0.6385184208488712
0.3456263101765258	0.9553355790548265	0.3794780847111909
0.0898993617213038	0.1605593093812618	0.4679419671899149
0.4205969995813304	0.8274008325970472	0.6763098520926030
0.6554675948960510	0.5330831466653910	0.7961130767470689
0.6745255450227732	0.6086265678320653	0.6454093791814887
0.1134497709676653	0.6885724066247551	0.6025950621626435
0.5480918378670622	0.1466511390059080	0.5713039542465795
0.2301783616882518	0.4942553941181979	0.3869603641632761

0.7774280615596619	0.0163987488242734	0.3837727994318843
0.3153376555362958	0.4328579743798839	0.6132606590521475
0.8444806799574615	0.4007488351746934	0.5752745081770951
0.5070038933830858	0.7386713108335948	0.3872587798252479
0.9824684245792754	0.7624149558182723	0.4050571399608344
0.5707607917130832	0.8894675244108092	0.6107526735766526
0.5922633154162733	0.4375809538907249	0.5827673384059204
0.2629752155454214	0.7765374309231746	0.3826504139578633
0.2358030497563499	0.2248353858392825	0.3830938861911096
0.2170032831574995	0.9833378862157975	0.3828898818471413
0.7773228184212595	0.5143465160518998	0.4257174477212450
0.1108647842931284	0.1810634482724912	0.6116558003527425
0.5557450621184805	0.6552558682503602	0.5903641189399336
0.0180829451776454	0.2409379514181980	0.3962983047001059
0.4810877665005385	0.2638671254829389	0.4207582168095749
0.8249464822418640	0.9365549594698737	0.6144268986944339
0.3450389054894482	0.9029334898209739	0.6133629661961083
0.7602811568402718	0.7843218875160241	0.3972185980519462
0.7321594790884800	0.2178998787075276	0.4244217557508561
0.0726259422180054	0.9002857870697427	0.6095055538245358
0.0937796777489894	0.4455684665323419	0.5925187520594034
0.0104862841327272	0.5174884342172233	0.3997152757527621
0.0000490423333343	0.0032682962782021	0.3874084739802391
0.4862456404077560	0.4981646168116650	0.4033402834695906
0.5012080159679605	0.9878803212174794	0.3918382676957046
0.8341744010579057	0.6861983226991979	0.5989999069257872
0.3209698469313822	0.1525255346359338	0.5986438143071581
0.3335254117144121	0.6697161807238610	0.6099606567594360
0.8493194362771468	0.1728981798210914	0.6047532177883911
0.6283683274032977	0.5081452966055241	0.7221773173830388

CONTCAR@CO(111)

O In O C

1.0000000000000000

14.4443000000000001 0.0000000000000000 0.0000000000000000

-7.2221499999999996 12.5091307398835685 0.0000000000000000

0.0000000000000009 0.0000000000000016 15.0371000000000006

O In O C

47 32 2 1

Direct

0.1388050097309889 0.8128549830306960 0.3561728924374861

0.4699163618777577 0.4803514897102004 0.5395313709553557

0.7692306746574777	0.4911277709593492	0.5715177918148291
0.4282451659834560	0.8245020581392858	0.3514248104801709
0.2868771729647647	0.2759679982520060	0.6017341313610214
0.9298352556866187	0.5979202502767587	0.3623324014141252
0.4836487128508334	0.7452571771619437	0.5258081987935290
0.1570029073064564	0.0732443842055818	0.3197184986180298
0.1830375903628092	0.3339304115284193	0.3473074140001737
0.5131131101906027	0.9873334639396376	0.5376135407568237
0.5072724819787557	0.2777600182386774	0.5670083289132327
0.1751274564005781	0.6065493198717671	0.3565976897014197
0.7279900325876801	0.0185937350098510	0.6266560230478468
0.4031426524885629	0.3370353948900202	0.3554906868182625
0.2640071351072791	0.7594089571154571	0.5268443665506677
0.9325882698163935	0.0943571861338708	0.3243259017900103
0.6693192488398633	0.8553442319191672	0.3461304402739852
0.0080917905556850	0.5308665923375713	0.5424074914411783
0.7178762902039978	0.2296702644176017	0.5705789129368252
0.3970747594530999	0.5729445031568396	0.3523787089096918
-0.0093206419222960	0.7249643203056070	0.5685145487906461
0.6656043019016175	0.0699538110883701	0.3570357379680987
0.2559297308182384	0.5184236871294172	0.5261194762207989
0.9115015723322247	0.8435463673961369	0.3327206053443791
0.1859324841089546	0.8516588753008520	0.6516456765178884
0.8555476959327915	0.1762637669843016	0.4589968463620949
0.5619967551870478	0.1765086636235794	0.4212077078739185
0.9052026709906273	0.8466950082881347	0.6418220461480671
0.0525855680237521	0.3981099566747570	0.4298256604897477
0.4009419654165690	0.0699149887562156	0.6348639615123514
0.8413513953271333	0.9366779135398083	0.4703403955784104
0.1744501621285716	0.5975562387015430	0.6653970893466047
0.1465227136386830	0.3416911689908527	0.6408439223073911
0.8126963968843064	0.6774074182198458	0.4547964803173836
0.8250633464763277	0.3866461475268443	0.4238638478666510
0.1594171545760292	0.0630069241361786	0.6421517232739408
0.6017654257374625	0.6605762325937530	0.4293946004426911
0.9298144574762041	0.3354299947934212	0.6366711343339578
0.0742415351452973	0.9260051541745500	0.4692100222780747
0.4115431987357130	0.5855966361595029	0.6668793605112944
0.6645281026077021	0.8103096516972801	0.6322244291489872
0.3189636777411908	0.1436156186923498	0.4529099879692410
0.6114896275142461	0.4394135232571766	0.4226046811342338
0.9455998656833834	0.1015795991911868	0.6383658070486127
0.3454563454455175	0.9552164224667753	0.3902672654174085
0.0900756212077113	0.1603806637276400	0.4676172228217817

0.4215524214077780	0.8282013530273173	0.6749779944510235
0.1139346676632922	0.6888872475601364	0.6038677803602860
0.5499870583033497	0.1500907828221206	0.5701678905932995
0.2299687652987208	0.4947147847600782	0.3862687345625384
0.7782077145103229	0.0169080338485438	0.3829860641981263
0.3157271723714443	0.4332438438307615	0.6096363278035219
0.8461295606050395	0.4003427398267507	0.5739494495543140
0.5072296119807754	0.7397642006607049	0.3854183641741786
0.9833598099411320	0.7632953211766070	0.4041259523282074
0.5721089697278582	0.8895323426916258	0.6104400326157590
0.5973022204475451	0.4462046577822478	0.5749519389279117
0.2631024150783114	0.7767422944574792	0.3840404367500341
0.2368342120019973	0.2254165590973697	0.3831373600452639
0.2174752512982815	0.9839524359056171	0.3847222193676232
0.7796118596401923	0.5147475546073328	0.4228615720710653
0.1112138203121446	0.1808261865227698	0.6112570010272173
0.5570665335866067	0.6544779186744588	0.5866646000197978
0.0186574091387196	0.2410723735551591	0.3959614853141284
0.4832466690007547	0.2668083196051300	0.4197181957140274
0.8253716877184570	0.9363982597528896	0.6144321860035835
0.3470188054042730	0.9045878830498162	0.6106616689881447
0.7608742442371277	0.7845381851699620	0.3954014132761028
0.7333783320327861	0.2182917746605803	0.4234172017966021
0.0717264593561090	0.8991393942183735	0.6105624721550557
0.0948312001470583	0.4462485730469155	0.5937205092413728
0.0117905684575473	0.5177425330575316	0.3996253950982203
0.0004801001479248	0.0037081182048411	0.3876494624925278
0.4848297540598407	0.4985814284429065	0.3978167272467958
0.5021872672865030	0.9887514881426992	0.3929875340966922
0.8304697349716293	0.6843887948099463	0.5971997842953222
0.3219097632581335	0.1537382523191606	0.5977052634207959
0.3347433222592138	0.6701526105770500	0.6098688727750951
0.8495157297374428	0.1724585169476834	0.6049908947803984
0.5579033212741827	0.4901862108353061	0.8103749126310874
0.6684648737937090	0.6018629767032527	0.6302461015820183
0.5623154853850991	0.4514571059380968	0.7455063622025332