A systematic theoretical study of CO_2 hydrogenation towards methanol on Cu-based bimetallic catalysts: Role of CHO&CH_3OH descriptor in thermodynamic analysis

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Evaluation details

To assess the predictive performance, three metrics were employed, that was, the Pearson correlation coefficient (PCC), determination coefficient (R^2) and mean-average error (MAE). Of these, PCC was mathematically represented by Eq. (1):

$$PCC = \frac{Cov(x,y)}{\sigma_x \sigma_y} \tag{1}$$

where $Cov(X,Y)$ signified the covariance between variables x and y, while σ_x and σ_y were their respective standard deviations. R^2 was introduced to evaluate the fitting degree of the learning model, as recorded in Eq. (2):

$$R^2 = \frac{\sum_{i=1}^{n} (y_i - f_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{2}$$

where y_i and f_i referred to the true and predicted values, respectively. $\bar{y}$ denoted the mean of the true values, and a higher value of R^2 indicated a stronger fit of learning models. Besides that, MAE, an essential indicator for quantifying the disparity between predicted and actual values, was formulated in Eq. (3):

$$MAE = \frac{\sum_{i=1}^{n} |y_i - f_i|}{n} \tag{3}$$

Computational details of SISSO

Input file of SISSO

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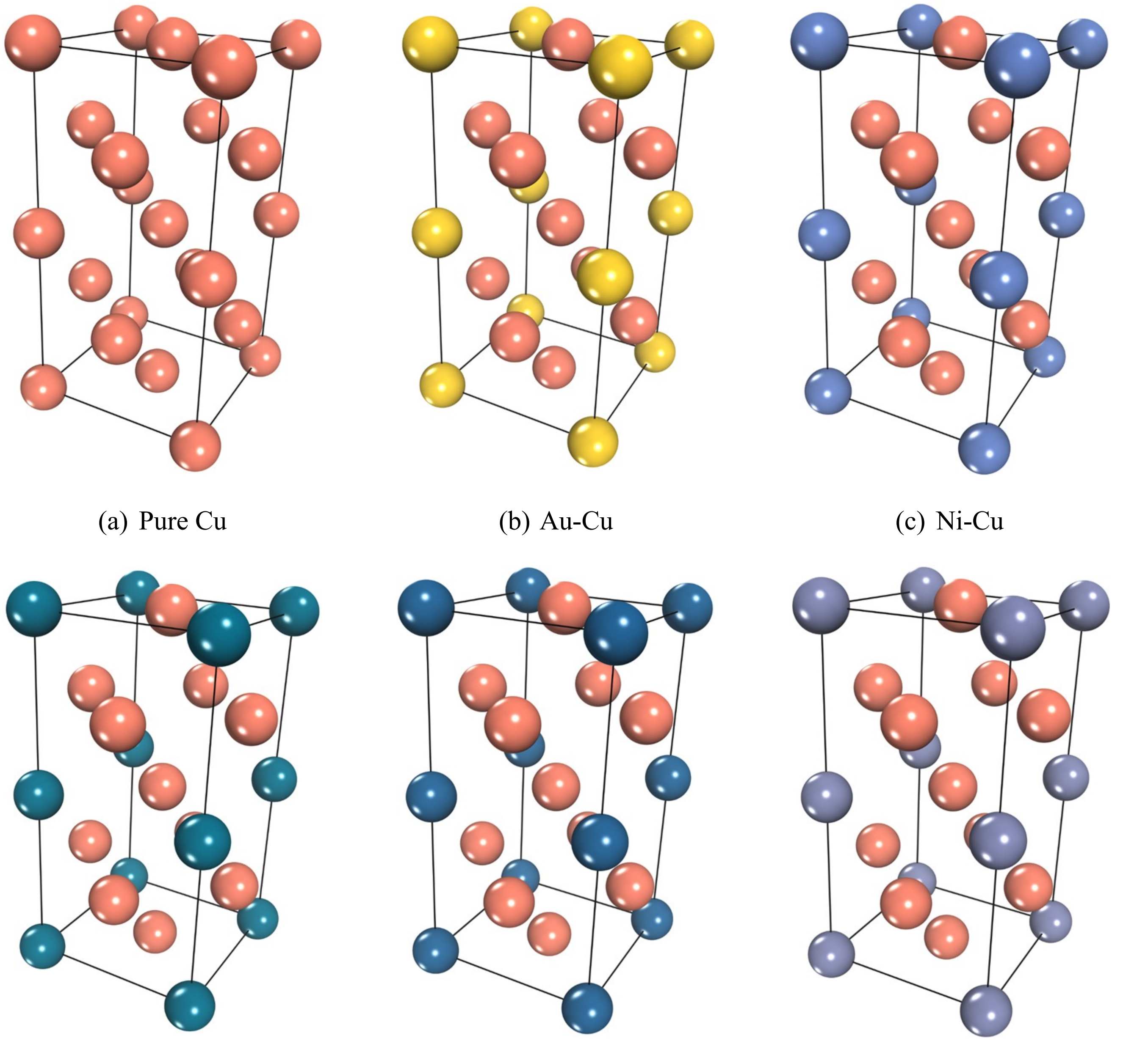
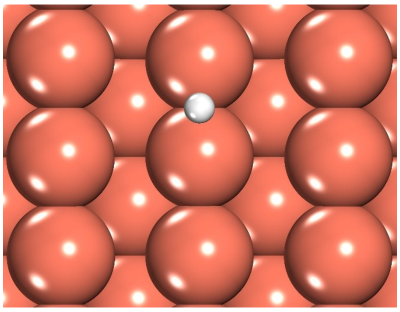
1. Figure captions



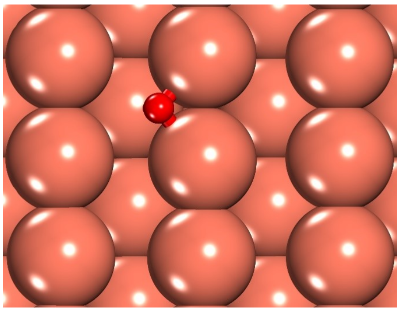
(a) Pure Cu (b) Au-Cu (c) Ni-Cu

(d) Pd-Cu (e) Pt-Cu (f) Zn-Cu

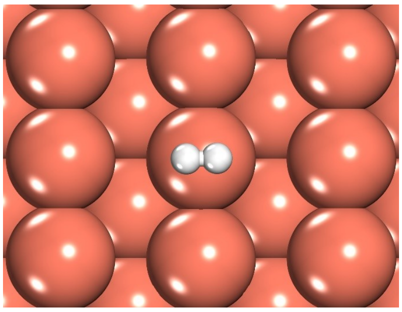
Fig. S1. Geometric structures of 1×1×2 crystal configuration for (a) pure Cu, (b) Au-Cu, (c) Ni-Cu, (d) Pd-Cu, (e) Pt-Cu and (f) Zn-Cu.



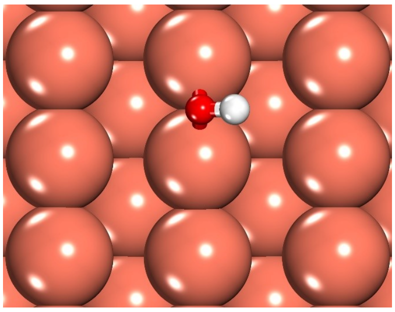
(a) H



(b) O



(c) H_2



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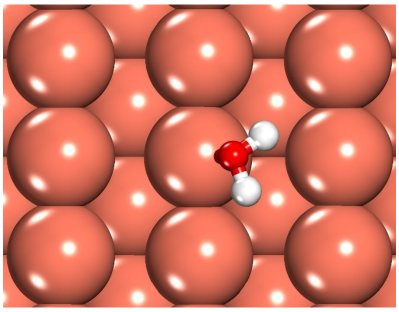
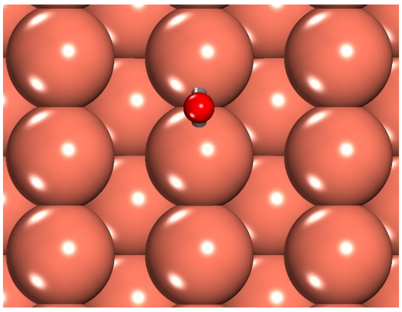
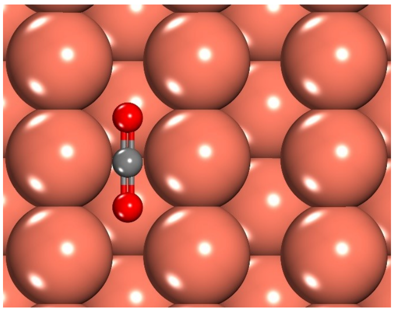


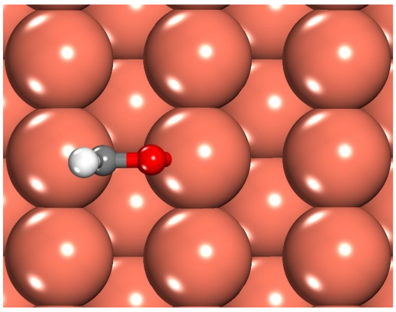
(e) H_2O



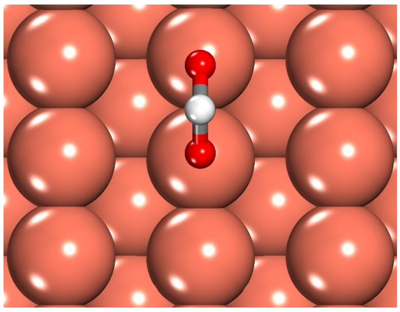
(f) CO



(g) CO_2



(h) CHO



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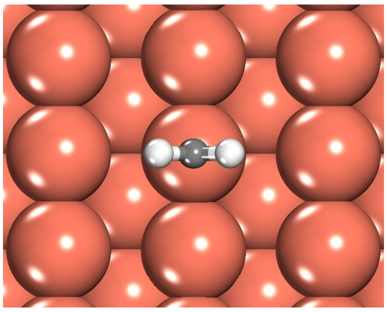

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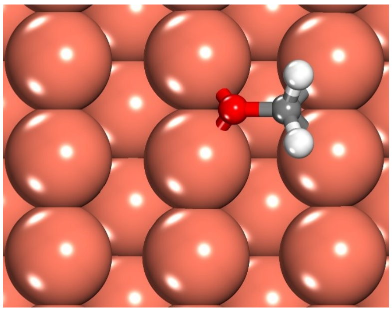
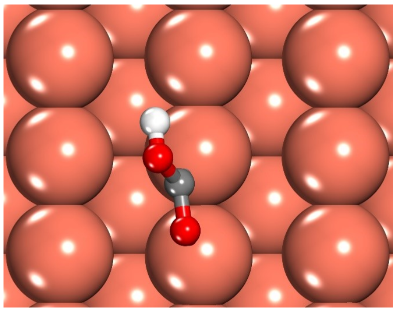
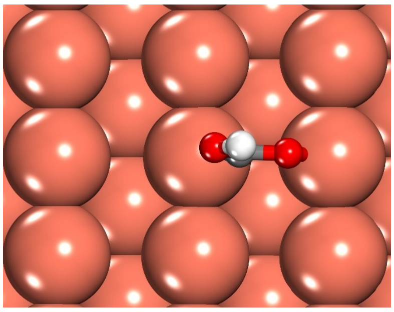


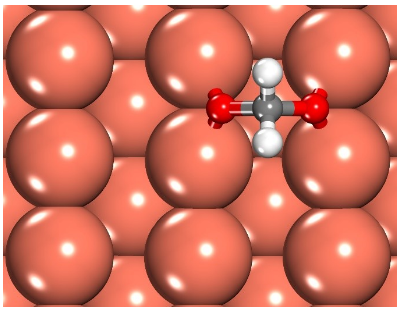
(k) bi-H_2CO



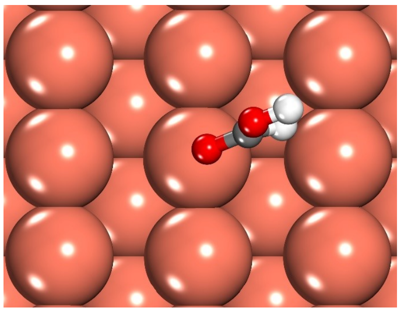
(l) trans-COOH



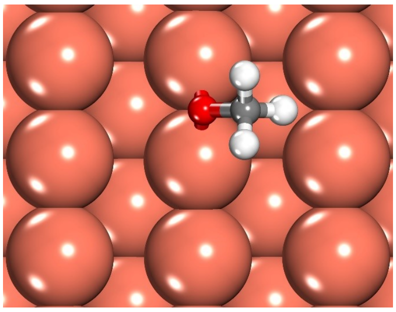
(m) cis-COOH



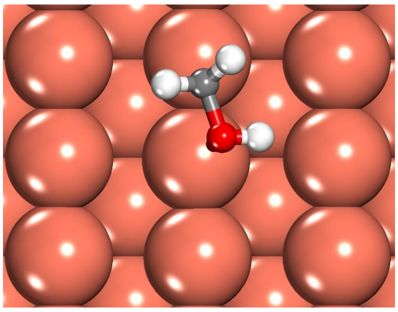
(n) H_2COO



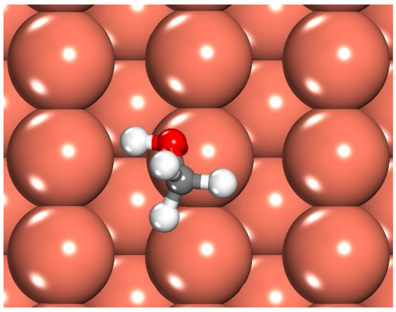
(o) HCOOH



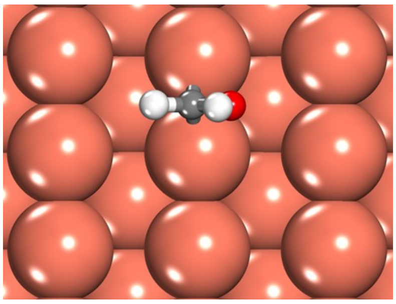
(p) CH_3O



(q) CH_2OH

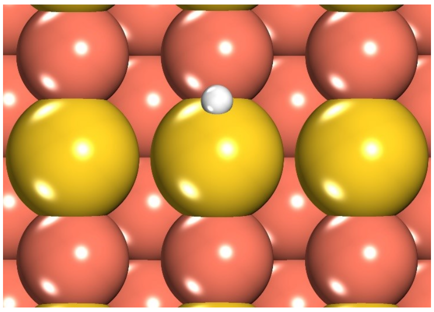


(r) CH_3OH

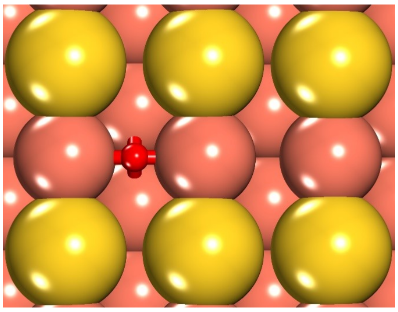


(s) CHOH

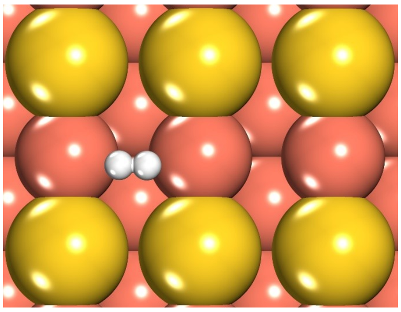
Fig. S2. Optimal configurations of reaction intermediates adsorbed on Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.



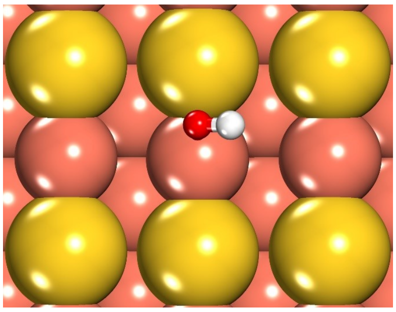
(a) H



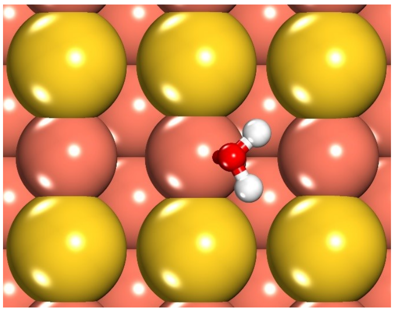
(b) O



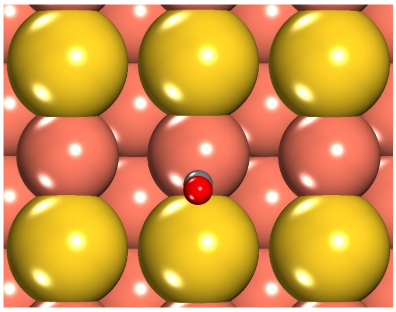
(c) H_2



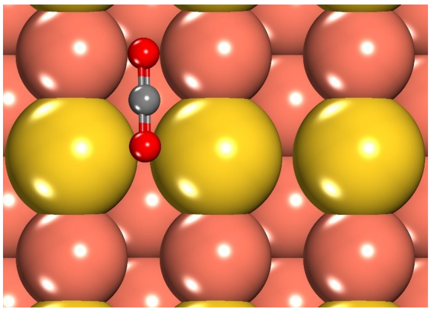
(d) OH



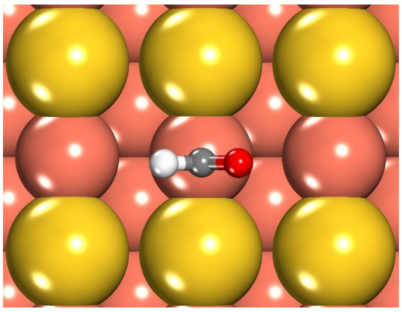
(e) H_2O



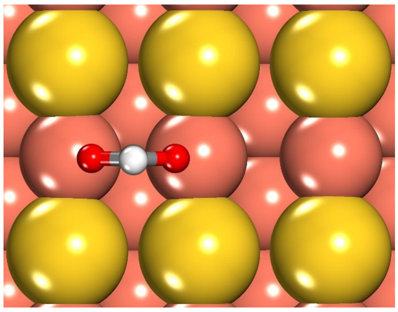
(f) CO



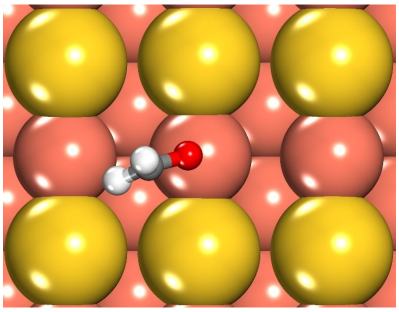
(g) CO_2



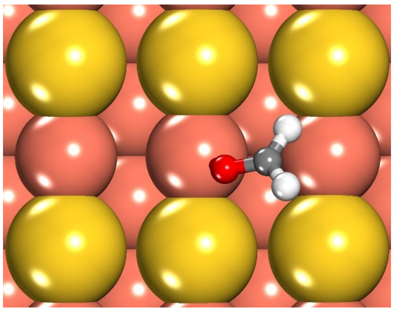
(h) CHO



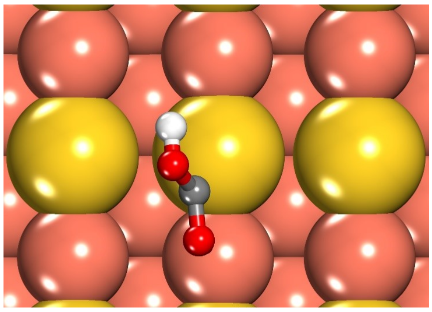
(i) bi-HCOO



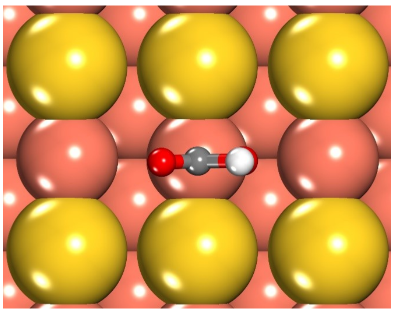
(j) mono-H_2CO



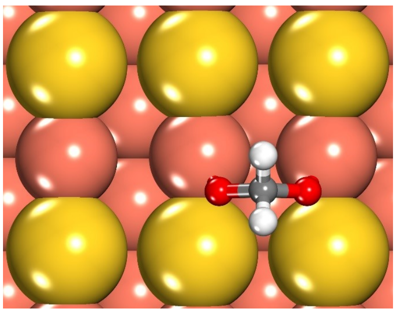
(k) bi-H_2CO



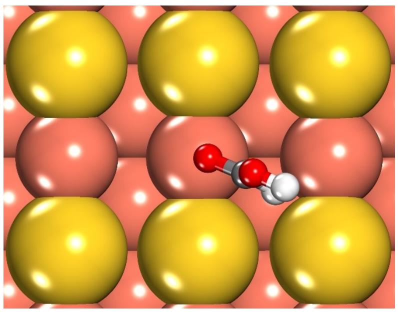
(l) trans-COOH



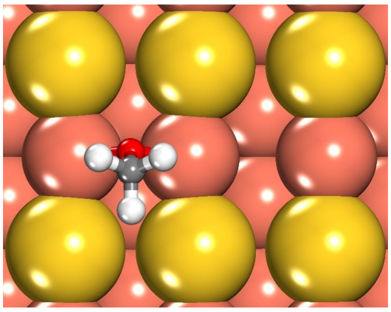
(m) cis-COOH



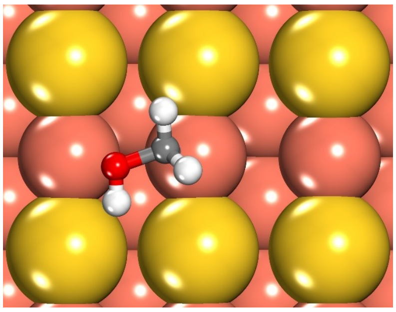
(n) H_2COO



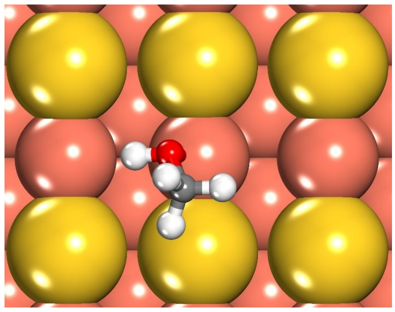
(o) HCOOH



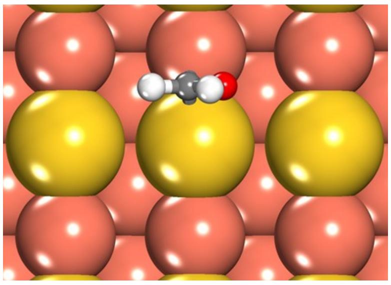
(p) CH_3O



(q) CH_2OH

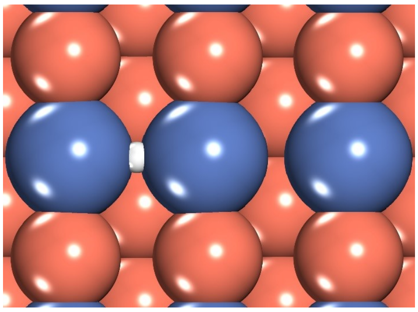


(r) CH_3OH

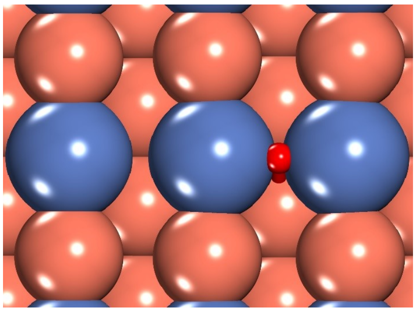


(s) CHOH

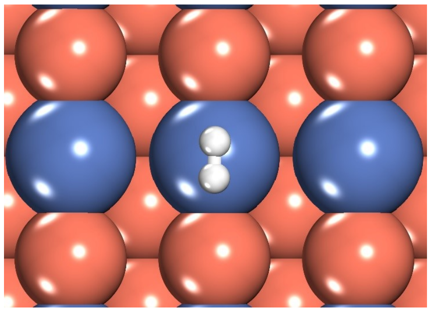
Fig. S3. Optimal configurations of reaction intermediates adsorbed on Au-Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.



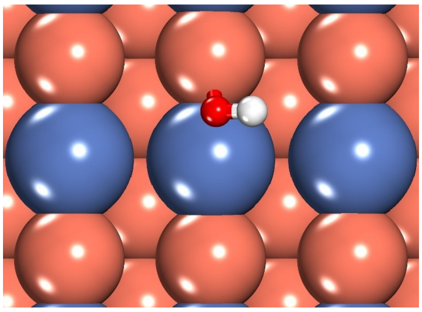
(a) H



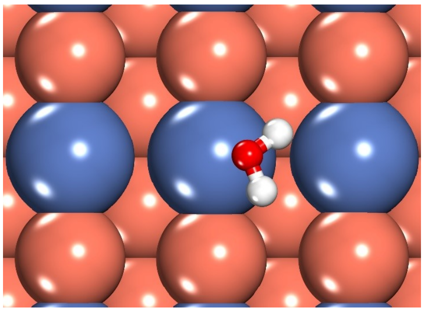
(b) O



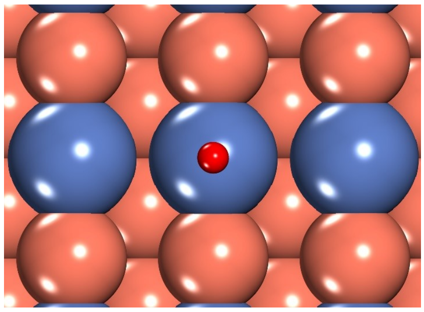
(c) H_2



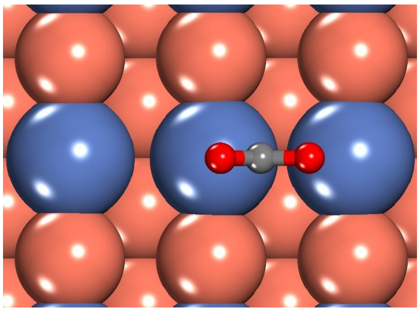
(d) OH



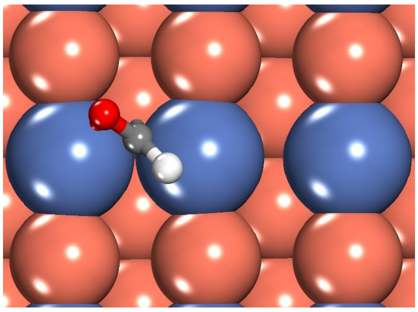
(e) H_2O



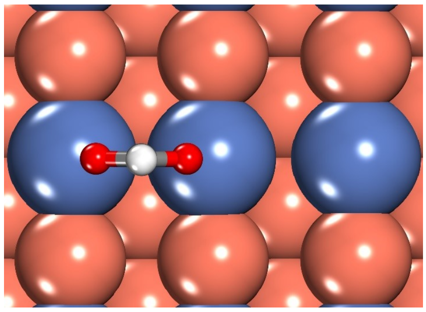
(f) CO



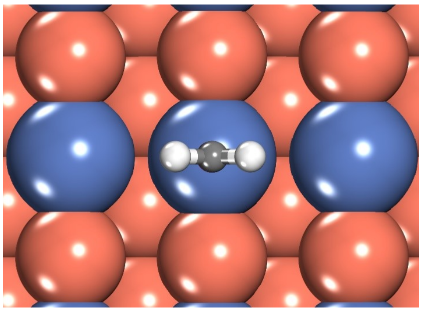
(g) CO_2



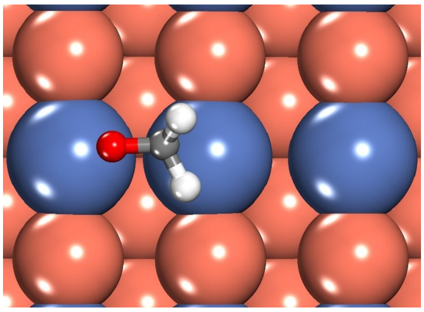
(h) CHO



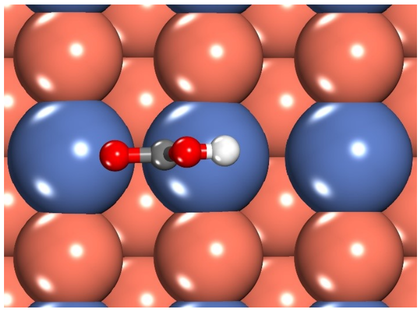
(i) bi-HCOO



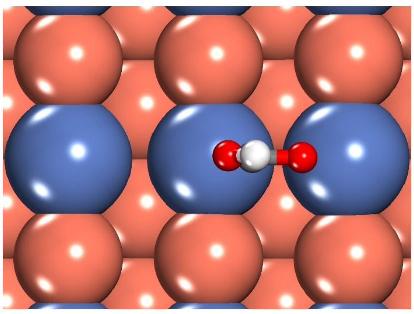
(j) mono-H_2CO



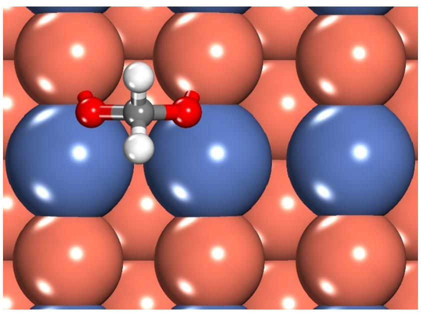
(k) bi-H_2CO



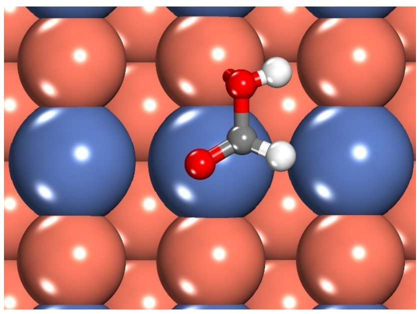
(l) trans-COOH



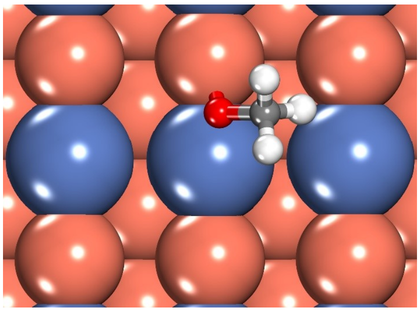
(m) cis-COOH



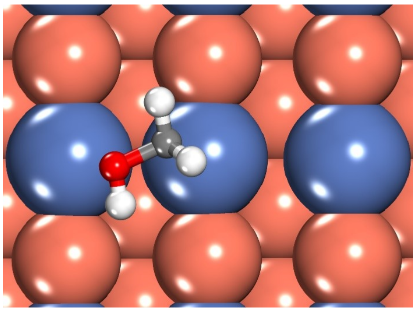
(n) H_2COO



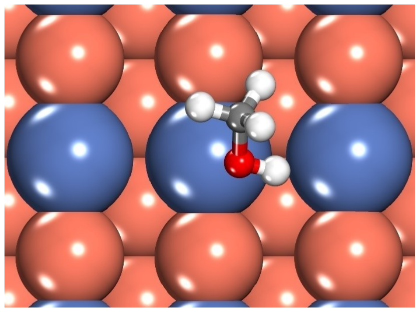
(o) HCOOH



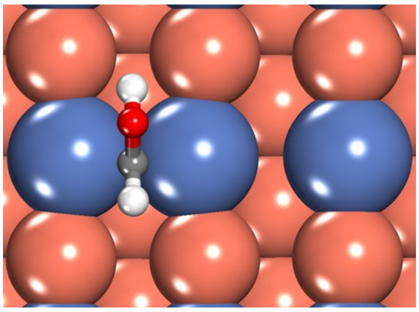
(p) CH_3O



(q) CH_2OH

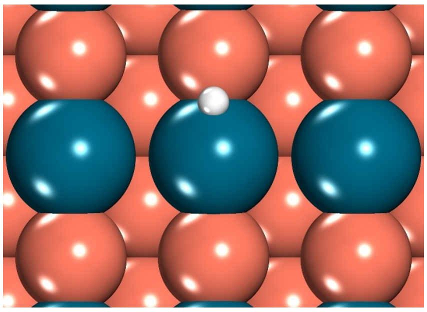


(r) CH_3OH

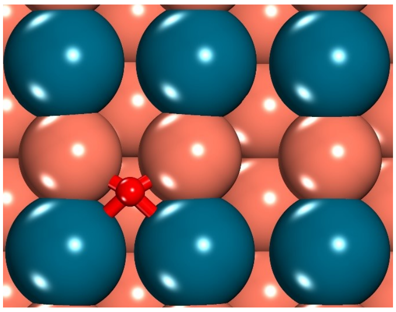


(s) CHOH

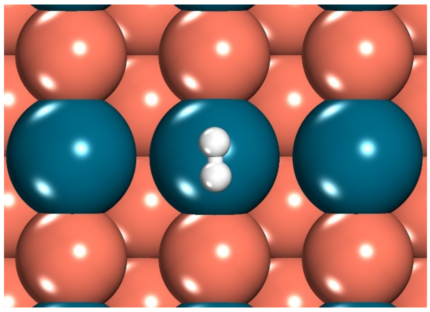
Fig. S4. Optimal configurations of reaction intermediates adsorbed on Ni-Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.



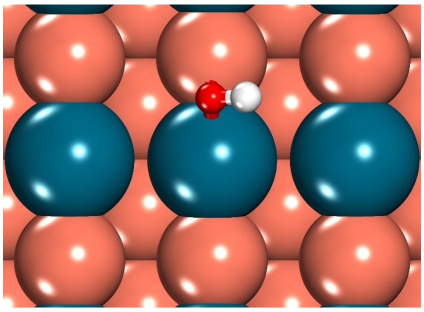
(a) H



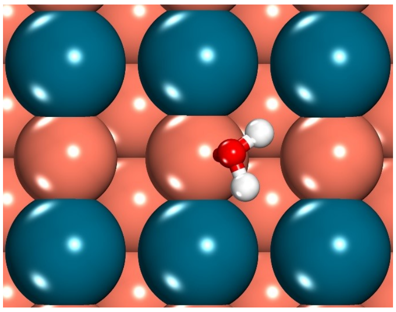
(b) O



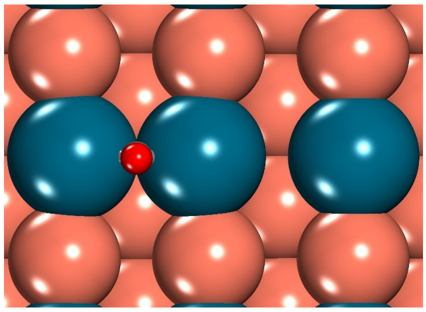
(c) H_2



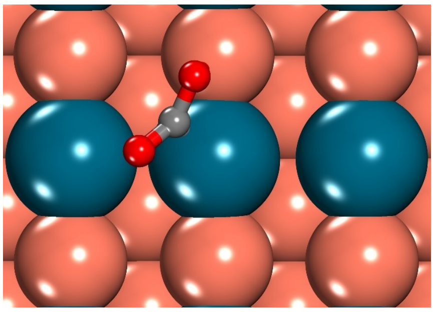
(d) OH



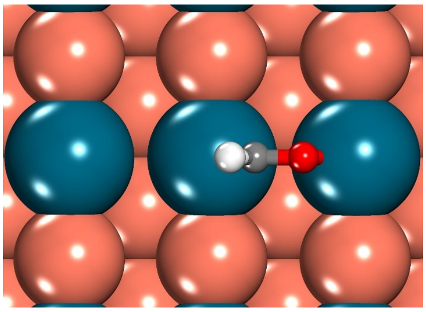
(e) H_2O



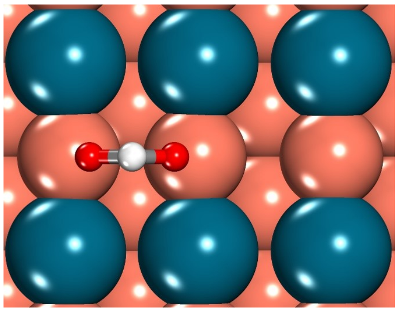
(f) CO



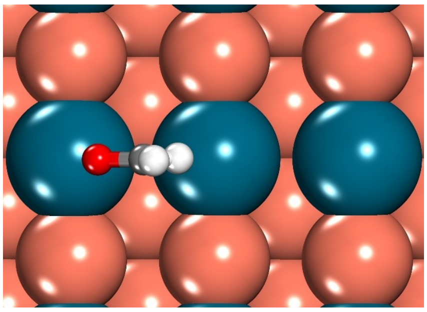
(g) CO_2



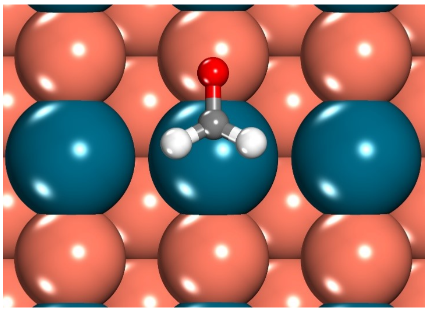
(h) CHO



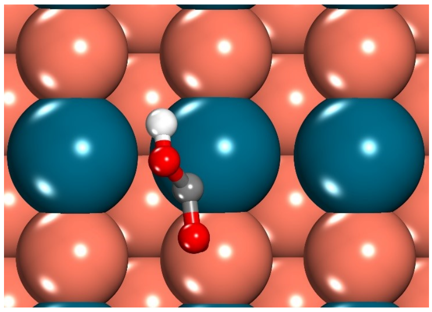
(i) bi-HCOO



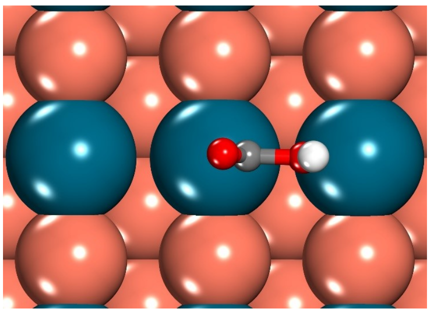
(j) mono-H_2CO



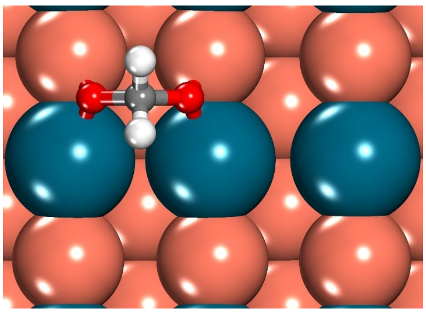
(k) bi-H_2CO



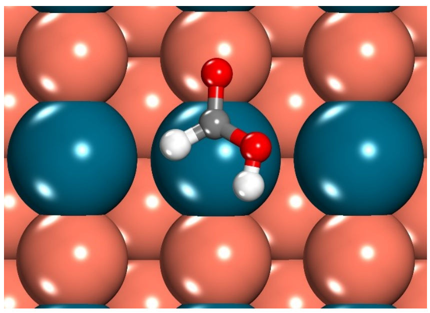
(l) trans-COOH



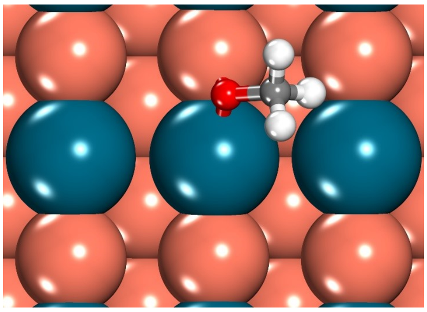
(m) cis-COOH



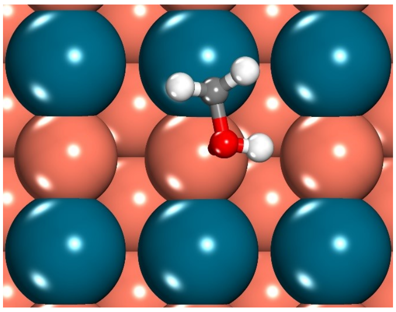
(n) H_2COO



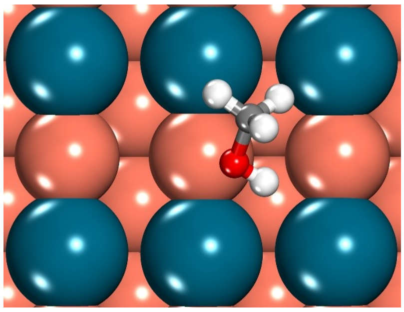
(o) HCOOH



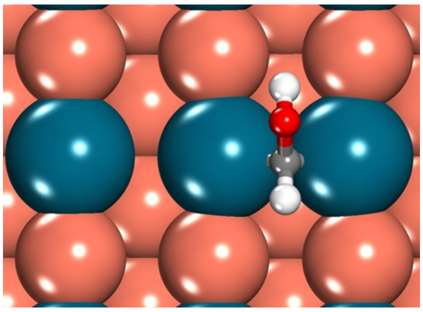
(p) CH_3O



(q) CH_2OH

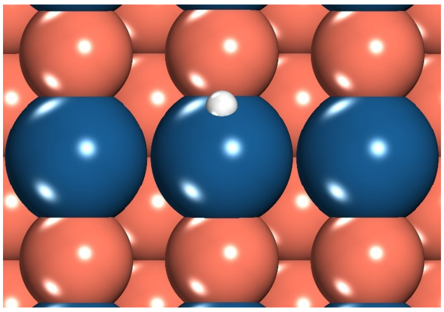


(r) CH_3OH

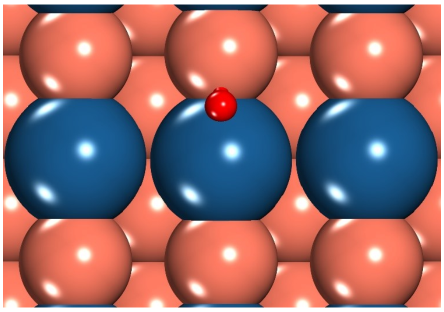


(s) CHOH

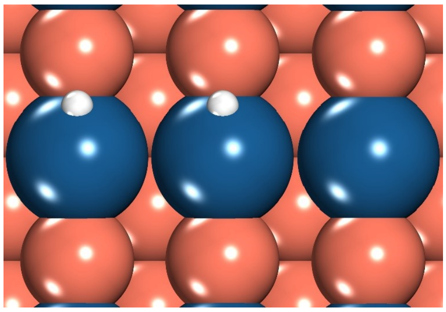
Fig. S5. Optimal configurations of reaction intermediates adsorbed on Pd-Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.



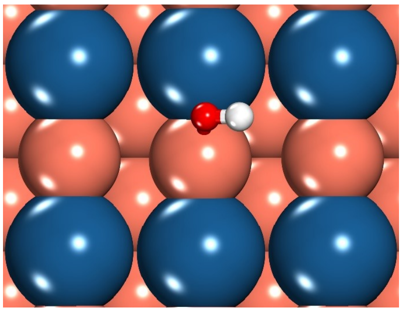
(a) H



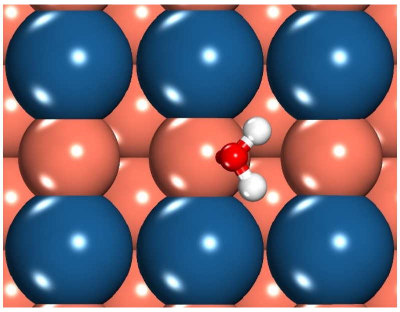
(b) O



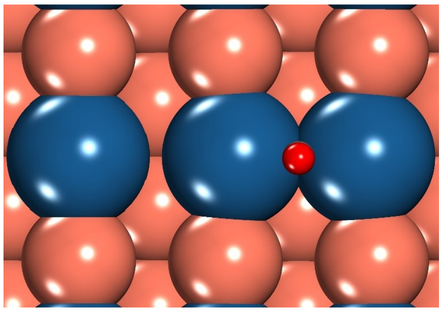
(c) H_2



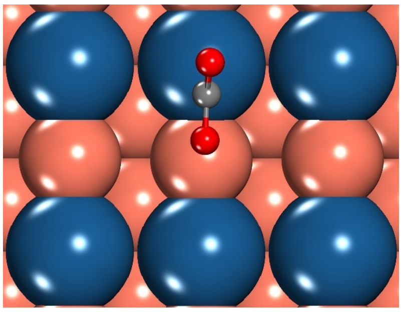
(d) OH



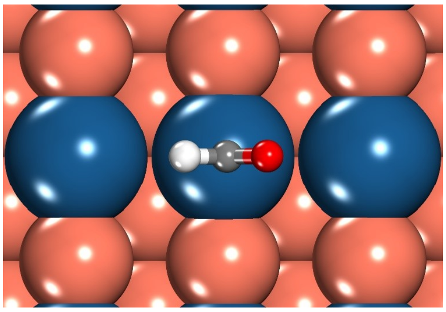
(e) H_2O



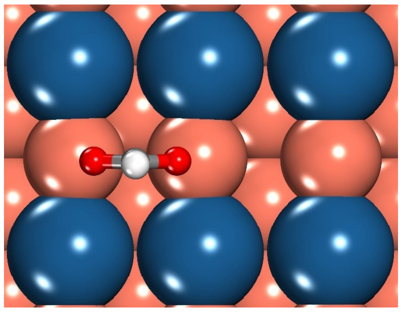
(f) CO



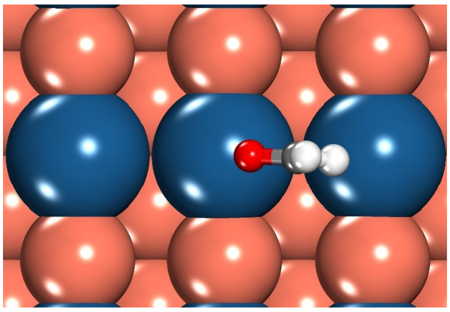
(g) CO_2



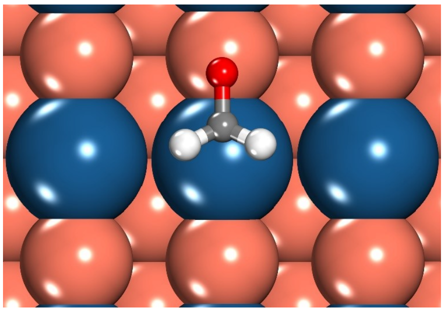
(h) CHO



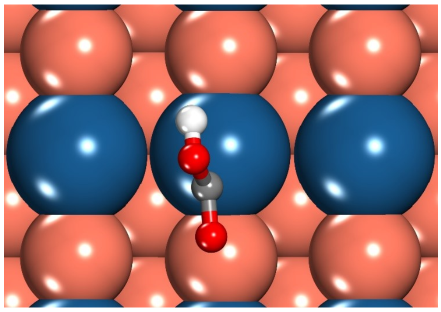
(i) bi-HCOO



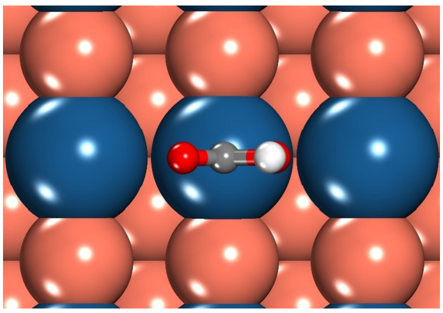
(j) mono-H_2CO



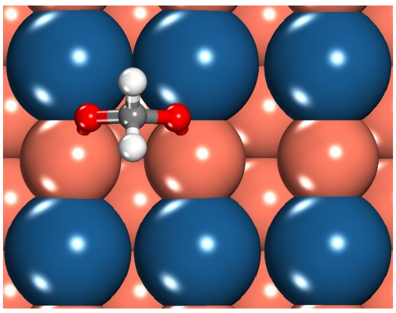
(k) bi-H_2CO



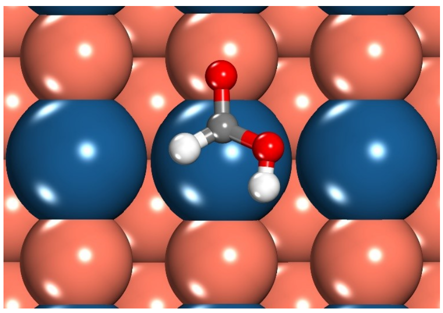
(l) trans-COOH



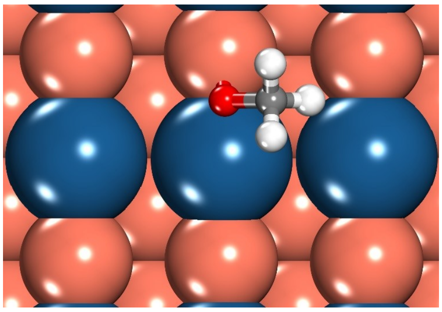
(m) cis-COOH



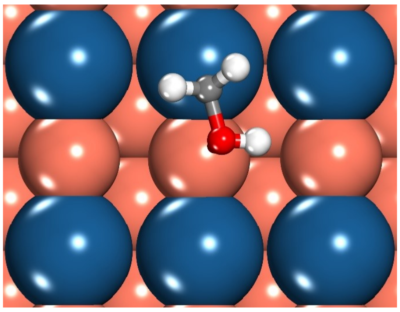
(n) H_2COO



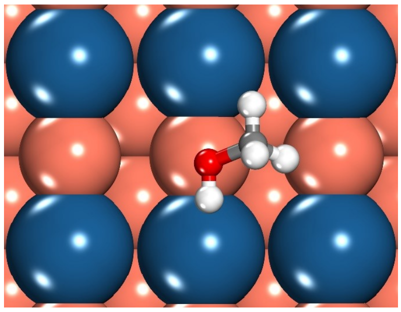
(o) HCOOH



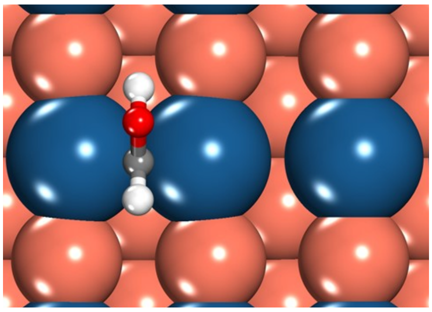
(p) CH_3O



(q) CH_2OH

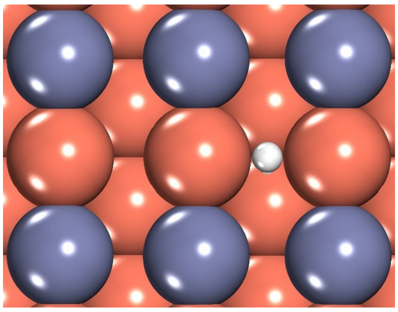


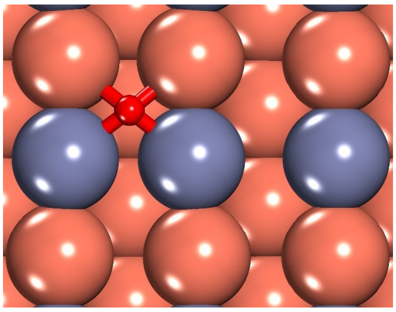
(r) CH_3OH

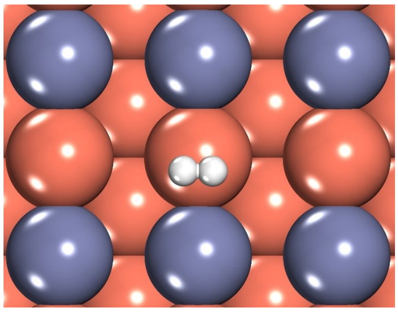


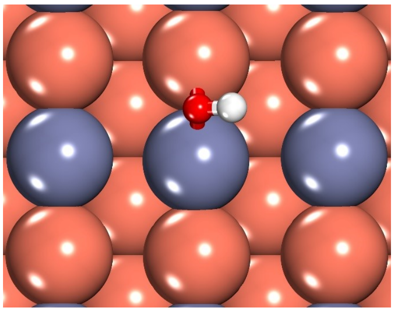
(s) CHOH

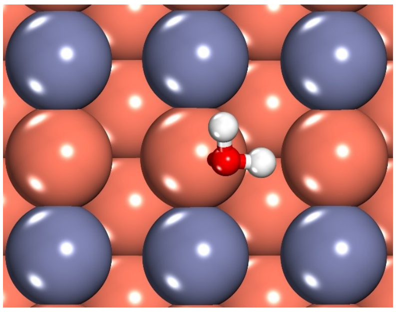
Fig. S6. Optimal configurations of reaction intermediates adsorbed on Pt-Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.

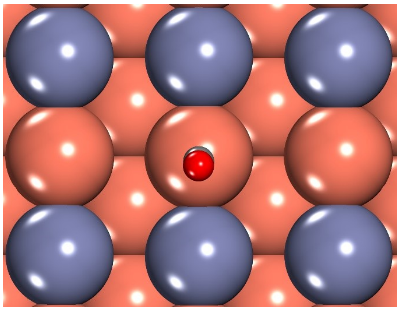

(a) H

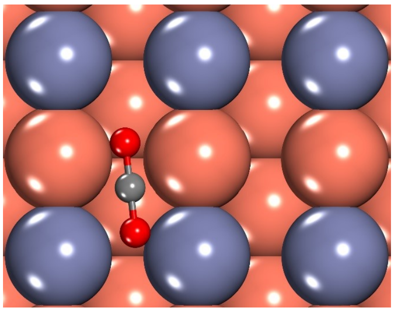

(b) O

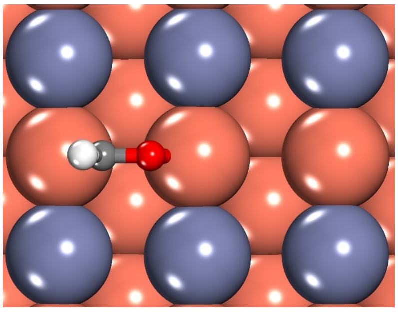

(c) H_2

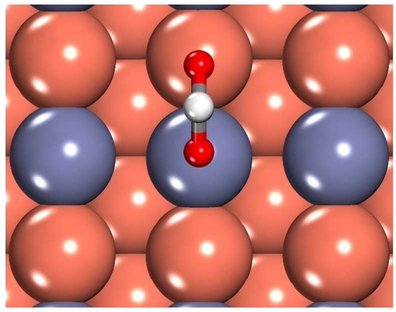

(d) OH

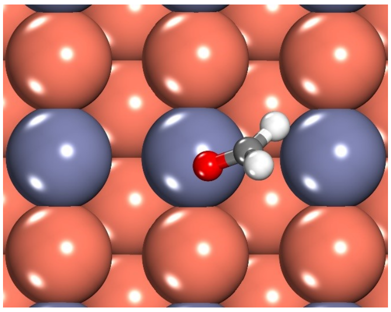

(e) H_2O

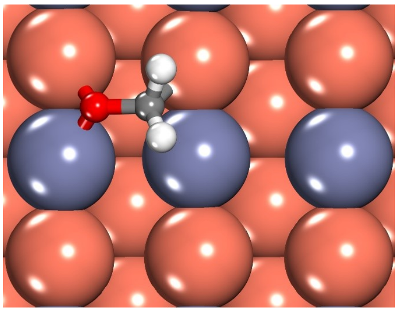

(f) CO

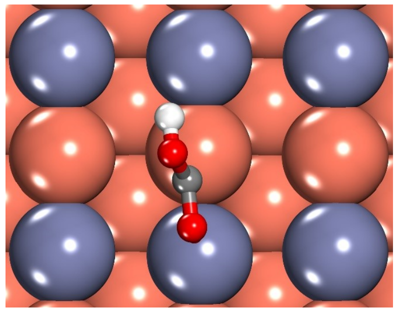

(g) CO_2

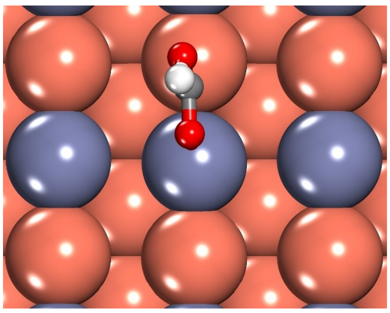

(h) CHO

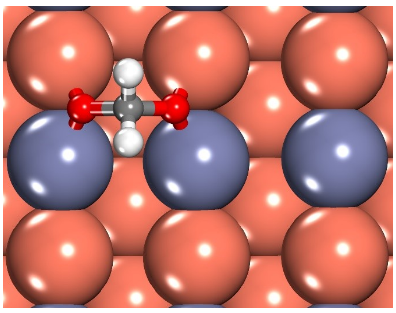

(i) bi-HCOO

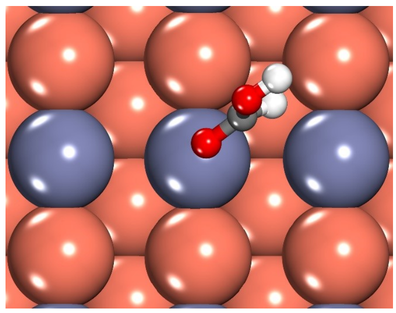

(j) mono-H_2CO

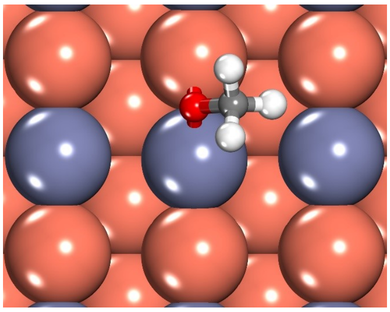

(k) bi-H_2CO


(l) trans-COOH

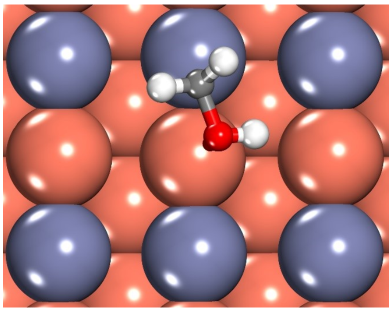

(m) cis-COOH


(n) H_2COO

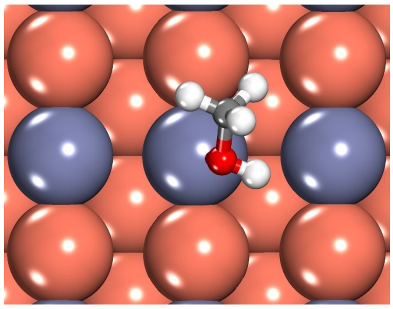

(o) HCOOH



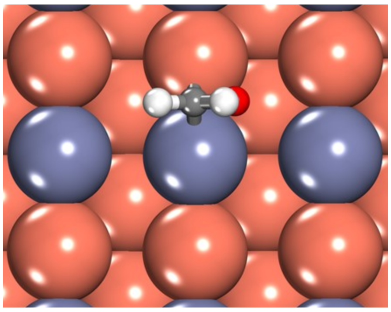
(p) CH_3O



(q) CH_2OH

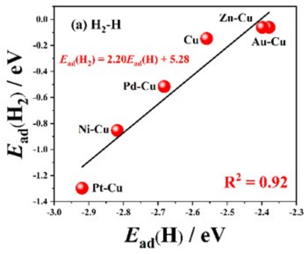


(r) CH_3OH

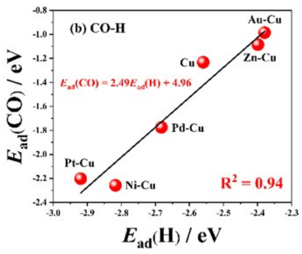


(s) CHOH

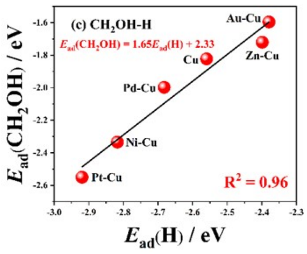
Fig. S7. Optimal configurations of reaction intermediates adsorbed on Zn-Cu substrate, containing (a) H*, (b) O*, (c) H_2*, (d) OH*, (e) H_2O*, (f) CO*, (g) CO_2*, (h) CHO*, (i) bi-HCOO*, (j) mono-H_2CO*, (k) bi-H_2CO*, (l) trans-COOH*, (m) cis-COOH*, (n) H_2COO*, (o) HCOOH*, (p) CH_3O*, (q) CH_2OH*, (r) CH_3OH* and (s) CHOH.



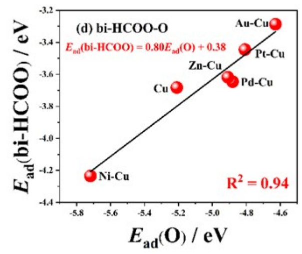
(a) $H_2 \sim H$



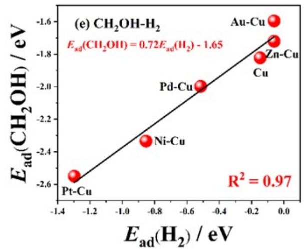
(b) $CO \sim H$



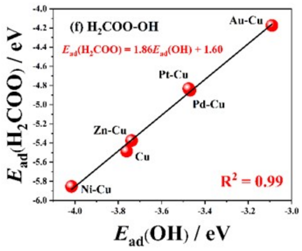
(c) $CH_2OH \sim H$



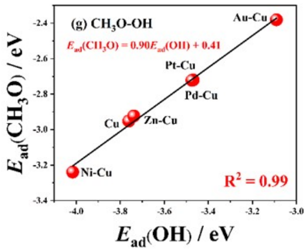
(d) bi-HCOO ~ O



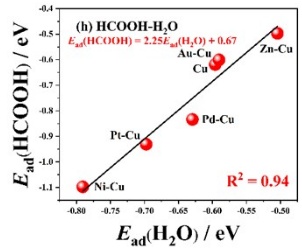
(e) $CH_2OH \sim H_2$



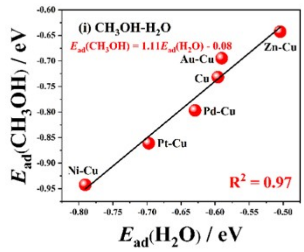
(f) $H_2COO \sim OH$



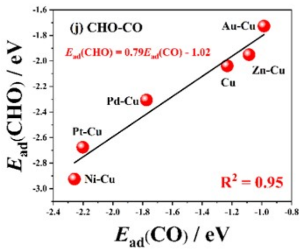
(g) $CH_3O \sim OH$



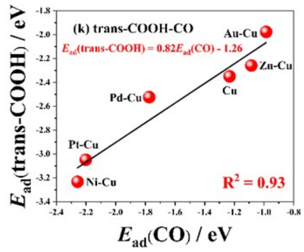
(h) $HCOOH \sim H_2O$



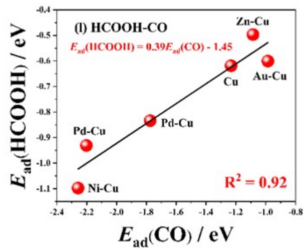
(i) $CH_3OH \sim H_2O$



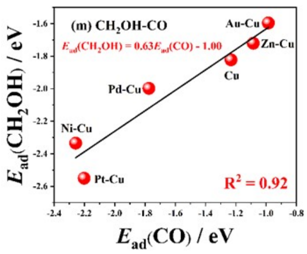
(j) $CHO \sim CO$



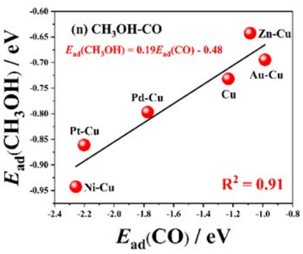
(k) trans-COOH ~ CO



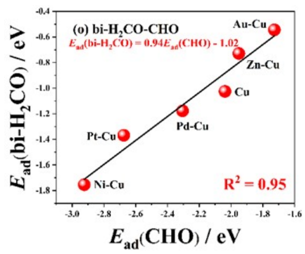
(l) $HCOOH \sim CO$



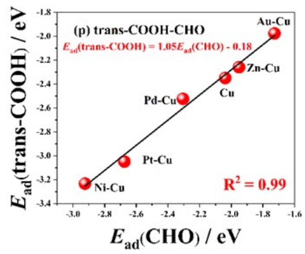
(m) $CH_2OH \sim CO$



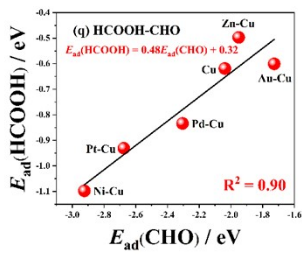
(n) $CH_3OH \sim CO$



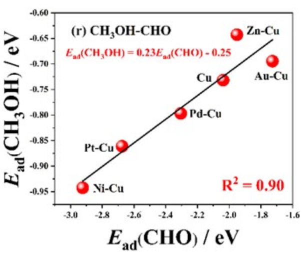
(o) bi-$H_2CO \sim CHO$



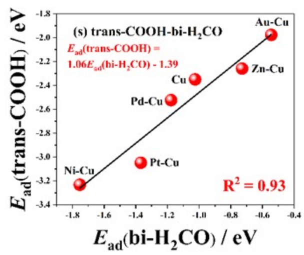
(p) trans-COOH ~ CHO



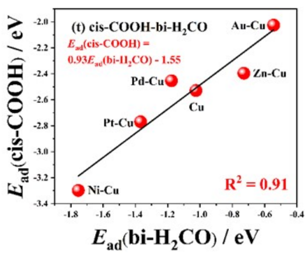
(q) $HCOOH \sim CHO$



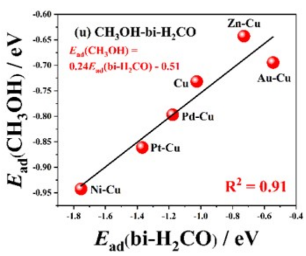
(r) $CH_3OH \sim CHO$



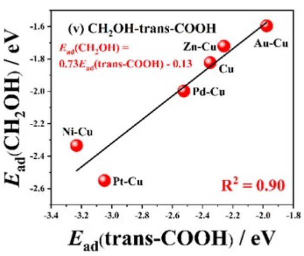
(s) trans-COOH ~ bi-H_2CO



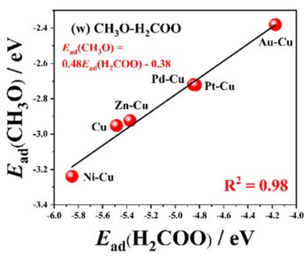
(t) cis-COOH ~ bi-H_2CO



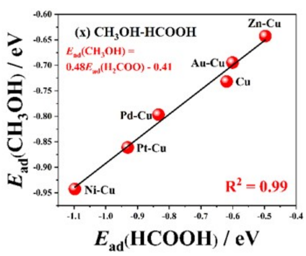
(u) $CH_3OH \sim$ bi-H_2CO



(v) $CH_2OH \sim$ trans-COOH



(w) $CH_3O \sim H_2COO$



(x) $CH_3OH \sim HCOOH$

Fig. S8. Highly correlated scaling relationships of adsorption energy between different reaction intermediates (greater than 0.9) during methanol synthesis, including (a) H_2 ~ H, (b) CO ~ H, (c) CH_2OH ~ H, (d) bi-HCOO ~ O, (e) CH_2OH ~ H_2, (f) H_2COO ~ OH, (g) CH_3O ~ OH, (h) HCOOH ~ H_2O, (i) CH_3OH ~ H_2O, (j) CHO ~ CO, (k) trans-COOH ~ CO, (l) HCOOH ~ CO, (m) CH_2OH ~ CO, (n) CH_3OH ~ CO, (o) bi-H_2CO ~ CHO, (p) trans-COOH ~ CHO, (q) HCOOH ~ CHO, (r) CH_3OH ~ CHO, (s) trans-COOH ~ bi-H_2CO, (t) cis-COOH ~ bi-H_2CO, (u) CH_3OH ~ bi-H_2CO, (v) CH_2OH ~ trans-COOH, (w) CH_3O ~ H_2COO and (x) CH_3OH ~ HCOOH.

2. Table captions

Table S1. Summary of determination coefficients for adsorption energy between different intermediate descriptors on Cu-based substrates.

Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2
O ~ H	0.16	H_2 ~ O	0.06	OH ~ H_2	0.03	H_2O ~ OH	0.13	CO ~ H_2O	0.79	CO_2 ~ CO	0.77	CHO ~ CO_2	0.87
H_2 ~ H	0.92	OH ~ O	0.79	H_2O ~ H_2	0.62	CO ~ OH	0.16	CO_2 ~ H_2O	0.88	CHO ~ CO	0.95	bi-HCOO ~ CO_2	0.56
OH ~ H	0.11	H_2O ~ O	0.40	CO ~ H_2	0.88	CO_2 ~ OH	0.27	CHO ~ H_2O	0.80	bi-HCOO ~ CO	0.29	mono-H_2CO ~ CO_2	0.87
H_2O ~ H	0.70	CO ~ O	0.24	CO_2 ~ H_2	0.55	CHO ~ OH	0.32	bi-HCOO ~ H_2O	0.38	mono-H_2CO ~ CO	0.61	bi-H_2CO ~ CO_2	0.82
CO ~ H	0.94	CO_2 ~ O	0.51	CHO ~ H_2	0.78	bi-HCOO ~ OH	0.78	mono-H_2CO ~ H_2O	0.73	bi-H_2CO ~ CO	0.88	trans-COOH ~ CO_2	0.83
CO_2 ~ H	0.60	CHO ~ O	0.41	bi-HCOO ~ H_2	0.06	mono-H_2CO ~ OH	0.08	bi-H_2CO ~ H_2O	0.81	trans-COOH ~ CO	0.93	cis-COOH ~ CO_2	0.83
CHO ~ H	0.86	bi-HCOO ~ O	0.94	mono-H_2CO ~ H_2	0.41	bi-H_2CO ~ OH	0.41	trans-COOH ~ H_2O	0.77	cis-COOH ~ CO	0.71	H_2COO ~ CO_2	0.23
bi-HCOO ~ H	0.17	mono-H_2CO ~ O	0.27	bi-H_2CO ~ H_2	0.64	trans-COOH ~ OH	0.33	cis-COOH ~ H_2O	0.69	H_2COO ~ CO	0.12	HCOOH ~ CO_2	0.88
mono-H_2CO ~ H	0.39	bi-H_2CO ~ O	0.56	trans-COOH ~ H_2	0.80	cis-COOH ~ OH	0.63	H_2COO ~ H_2O	0.10	HCOOH ~ CO	0.92	CH_3O ~ CO_2	0.35
bi-H_2CO ~ H	0.81	trans-COOH ~ O	0.40	cis-COOH ~ H_2	0.48	H_2COO ~ OH	0.99	HCOOH ~ H_2O	0.94	CH_3O ~ CO	0.20	CH_2OH ~ CO_2	0.62
trans-COOH ~ H	0.87	cis-COOH ~ O	0.73	H_2COO ~ H_2	0.02	HCOOH ~ OH	0.13	CH_3O ~ H_2O	0.18	CH_2OH ~ CO	0.92	CH_3OH ~ CO_2	0.88
cis-COOH ~ H	0.61	H_2COO ~ O	0.78	HCOOH ~ H_2	0.73	CH_3O ~ OH	0.99	CH_2OH ~ H_2O	0.65	CH_3OH ~ CO	0.91		

H_2COO ~ H	0.09	HCOOH ~ O	0.33	CH_3O ~ H_2	0.05	CH_2OH ~ OH	0.12	CH_3OH ~ H_2O	0.97
HCOOH ~ H	0.81	CH_3O ~ O	0.84	CH_2OH ~ H_2	0.97	CH_3OH ~ OH	0.16		
CH_3O ~ H	0.15	CH_2OH ~ O	0.14	CH_3OH ~ H_2	0.72				
CH_2OH ~ H	0.96	CH_3OH ~ O	0.38						
CH_3OH ~ H	0.83								

Continue

Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2	Intermediate Pairing	R^2
bi-HCOO ~ CHO	0.46	mono-H_2CO ~ bi-HCOO	0.38	bi-H_2CO ~ mono-H_2CO	0.56	trans-COOH ~ bi-H_2CO	0.93	cis-COOH ~ trans-COOH	0.88	H_2COO ~ cis-COOH-	0.57
mono-H_2CO ~ CHO	0.64	bi-H_2CO ~ bi-HCOO	0.58	trans-COOH ~ mono-H_2CO	0.57	cis-COOH ~ bi-H_2CO	0.91	H_2COO ~ trans-COOH	0.28	HCOOH ~ cis-COOH-	0.70
bi-H_2CO ~ CHO	0.95	trans-COOH ~ bi-HCOO	0.43	cis-COOH ~ mono-H_2CO	0.51	H_2COO ~ bi-H_2CO	0.36	HCOOH ~ trans-COOH	0.85	CH_3O ~ cis-COOH-	0.69
trans-COOH ~ CHO	0.99	cis-COOH ~ bi-HCOO	0.73	H_2COO ~ mono-H_2CO	0.05	HCOOH ~ bi-H_2CO	0.87	CH_3O ~ trans-COOH	0.39	CH_2OH ~ cis-COOH-	0.63
cis-COOH ~ CHO	0.88	H_2COO ~ bi-HCOO	0.76	HCOOH ~ mono-H_2CO	0.77	CH_3O ~ bi-H_2CO	0.48	CH_2OH ~ trans-COOH	0.90	CH_3OH ~ cis-COOH-	0.75
H_2COO ~ CHO	0.26	HCOOH ~ bi-HCOO	0.37	CH_3O ~ mono-H_2CO	0.13	CH_2OH ~ bi-H_2CO	0.76	CH_3OH ~ trans-COOH	0.87		
HCOOH ~ CHO	0.90	CH_3O ~ bi-HCOO	0.84	CH_2OH ~ mono-H_2CO	0.41	CH_3OH ~ bi-H_2CO	0.91				

CH_3O ~ CHO	0.38	CH_2OH ~ bi-HCOO	0.15	CH_3OH ~ mono-H_2CO	0.70
CH_2OH ~ CHO	0.87	CH_3OH ~ bi-HCOO	0.24		
CH_3OH ~ CHO	0.90				

Continue

Intermediate Pairing	**R^2**	**Intermediate Pairing**	**R^2**	**Intermediate Pairing**	**R^2**	**Intermediate Pairing**	**R^2**
HCOOH ~ H_2COO	0.10	CH_3O ~ HCOOH	0.18	CH_2OH ~ CH_3O-	0.16	CH_3OH ~ CH_2OH	0.77
CH_3O ~ H_2COO	0.98	CH_2OH ~ HCOOH	0.76	CH_3OH ~ CH_3O-	0.22		
CH_2OH ~ H_2COO	0.09	CH_3OH ~ HCOOH	0.99				
CH_3OH ~ H_2COO	0.13						

Table S2. Summary of average determination coefficients for adsorption energy between dual intermediate descriptors and all intermediates involved in CO_2 hydrogenation.

IM combination	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**
H&H	0.61	H&O	0.68	H&H_2	0.57	H&OH	0.63	H&H_2O	0.66	H&CO	0.67
O&H	0.68	O&O	0.50	O&H_2	0.74	O&OH	0.48	O&H_2O	0.57	O&CO	0.74
H_2&H	0.57	H_2&O	0.74	H_2&H_2	0.54	H_2&OH	0.68	H_2&H_2O	0.59	H2&CO	0.63
OH&H	0.63	OH&O	0.48	OH&H_2	0.68	OH&OH	0.41	OH&H_2O	0.55	OH&CO	0.72
H_2O&H	0.66	H_2O&O	0.57	H_2O&H_2	0.59	H_2O&OH	0.55	H_2O&H_2O	0.64	H2O&CO	0.69
CO&H	0.67	CO&O	0.74	CO&H_2	0.63	CO&OH	0.72	CO&H_2O	0.69	CO&CO	0.68
CO_2&H	0.73	CO_2&O	0.65	CO_2&H_2	0.67	CO_2&OH	0.67	CO_2&H_2O	0.69	CO_2&CO	0.72
CHO&H	0.71	CHO&O	0.72	CHO&H_2	0.66	CHO&OH	0.70	CHO&H_2O	0.74	CHO&CO	0.71
bi-HCOO&H	0.71	bi-HCOO&O	0.51	bi-HCOO&H_2	0.74	bi-HCOO&OH	0.49	bi-HCOO&H_2O	0.60	bi-HCOO&CO	0.74
mono-H_2CO&H	0.68	mono-H_2CO&O	0.59	mono-H_2CO&H_2	0.61	mono-H_2CO&OH	0.59	mono-H_2CO&H_2O	0.59	mono-H_2CO&CO	0.69
bi-H_2CO&H	0.72	bi-H_2CO&O	0.68	bi-H_2CO&H_2	0.68	bi-H_2CO&OH	0.67	bi-H_2CO&H_2O	0.74	bi-H_2CO&CO	0.72
trans-COOH&H	0.70	trans-COOH&O	0.72	trans-COOH&H_2	0.65	trans-COOH&OH	0.69	trans-COOH&H_2O	0.73	trans-COOH&CO	0.71
cis-COOH&H	0.74	cis-COOH&O	0.64	cis-COOH&H_2	0.70	cis-COOH&OH	0.62	cis-COOH&H_2O	0.74	cis-COOH&CO	0.74
H_2COO&H	0.53	H_2COO&O	0.45	H_2COO&H_2	0.65	H_2COO&OH	0.39	H_2COO&H_2O	0.46	H_2COO&CO	0.67
HCOOH&H	0.68	HCOOH&O	0.66	HCOOH&H_2	0.62	HCOOH&OH	0.67	HCOOH&H_2O	0.68	HCOOH&CO	0.69

CH_3O&H	0.67	CH_3O&O	0.50	CH_3O&H_2	0.69	CH_3O&OH	0.43	CH_3O&H_2O	0.59	CH_3O&CO	0.73
CH_2OH&H	0.61	CH_2OH&O	0.73	CH_2OH&H_2	0.57	CH_2OH&OH	0.66	CH_2OH&H_2O	0.65	CH_2OH&CO	0.66

Continue

IM combination	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**	**IM combination**	**R^2**
H&CO_2	0.73	H&CHO	0.71	H&bi-HCOO	0.71	H&mono-H_2CO	0.68	H&bi-H_2CO	0.72	H&trans-COOH	0.70
O&CO_2	0.65	O&CHO	0.72	O&bi-HCOO	0.51	O&mono-H_2CO	0.59	O&bi-H_2CO	0.68	O&trans-COOH	0.72
H_2&CO_2	0.67	H_2&CHO	0.66	H_2&bi-HCOO	0.74	H_2&mono-H_2CO	0.61	H_2&bi-H_2CO	0.68	H_2&trans-COOH	0.65
OH&CO_2	0.67	OH&CHO	0.70	OH&bi-HCOO	0.49	OH&mono-H_2CO	0.59	OH&bi-H_2CO	0.67	OH&trans-COOH	0.69
H_2O&CO_2	0.69	H_2O&CHO	0.74	H_2O&bi-HCOO	0.60	H_2O&mono-H_2CO	0.59	H_2O&bi-H_2CO	0.74	H_2O&trans-COOH	0.73
CO&CO_2	0.72	CO&CHO	0.71	CO&bi-HCOO	0.74	CO&mono-H_2CO	0.69	CO&bi-H_2CO	0.72	CO&trans-COOH	0.71
CO_2&CO_2	0.68	CO_2&CHO	0.74	CO_2&bi-HCOO	0.66	CO_2&mono-H_2CO	0.64	CO_2&bi-H_2CO	0.74	CO_2&trans-COOH	0.74
CHO&CO_2	0.74	CHO&CHO	0.73	CHO&bi-HCOO	0.73	CHO&mono-H_2CO	0.72	CHO&bi-H_2CO	0.74	CHO&trans-COOH	0.73
bi-HCOO&CO_2	0.66	bi-HCOO&CHO	0.73	bi-HCOO&bi-HCOO	0.52	bi-HCOO&mono-H_2CO	0.59	bi-HCOO&bi-H_2CO	0.70	bi-HCOO&trans-COOH	0.73
mono-H_2CO&CO_2	0.64	mono-H_2CO&CHO	0.72	mono-H_2CO&bi-HCOO	0.59	mono-H_2CO&mono-H_2CO	0.51	mono-H_2CO&bi-H_2CO	0.74	mono-H_2CO&trans-COOH	0.73
bi-H_2CO&CO_2	0.74	bi-H_2CO&CHO	0.74	bi-H_2CO&bi-HCOO	0.70	bi-H_2CO&mono-H_2CO	0.74	bi-H_2CO&bi-H_2CO	0.74	bi-H_2CO&trans-COOH	0.74
trans-COOH&CO_2	0.74	trans-COOH&CHO	0.73	trans-COOH&bi-HCOO	0.73	trans-COOH&mono-H_2CO	0.73	trans-COOH&bi-H_2CO	0.74	trans-COOH&trans-COOH	0.72
cis-COOH&CO_2	0.73	cis-COOH&CHO	0.75	cis-COOH&bi-HCOO	0.66	cis-COOH&mono-H_2CO	0.73	cis-COOH&bi-H_2CO	0.74	cis-COOH&trans-COOH	0.74
H_2COO&CO_2	0.59	H_2COO&CHO	0.62	H_2COO&bi-HCOO	0.45	H_2COO&mono-H_2CO	0.51	H_2COO&bi-H_2CO	0.59	H_2COO&trans-COOH	0.62
HCOOH&CO_2	0.70	HCOOH&CHO	0.73	HCOOH&bi-HCOO	0.67	HCOOH&mono-H_2CO	0.64	HCOOH&bi-H_2CO	0.73	HCOOH&trans-COOH	0.73

CH_3O&CO_2	0.68	CH_3O&CHO	0.71	CH_3O&bi-HCOO	0.50	CH_3O&mono-H_2CO	0.62	CH_3O&bi-H_2CO	0.69	CH_3O&trans-COOH	0.71
CH_2OH&CO_2	0.71	CH_2OH&CHO	0.69	CH_2OH&bi-HCOO	0.74	CH_2OH&mono-H_2CO	0.67	CH_2OH&bi-H_2CO	0.71	CH_2OH&trans-COOH	0.68

Continue

IM combination	R^2	IM combination	R^2	IM combination	R^2	IM combination	R^2	IM combination	R^2	IM combination	R^2
H&cis-COOH	0.74	H&H_2COO	0.54	H&HCOOH	0.67	H&CH_3O	0.67	H&CH_2OH	0.61	H&CH_3OH	0.66
O&cis-COOH	0.64	O&H_2COO	0.44	O&HCOOH	0.65	O&CH_3O	0.50	O&CH_2OH	0.73	O&CH_3OH	0.59
H_2&cis-COOH	0.70	H_2&H_2COO	0.65	H_2&HCOOH	0.62	H_2&CH_3O	0.69	H_2&CH_2OH	0.57	H_2&CH_3OH	0.59
OH&cis-COOH	0.62	OH&H_2COO	0.39	OH&HCOOH	0.67	OH&CH_3O	0.43	OH&CH_2OH	0.66	OH&CH_3OH	0.57
H_2O&cis-COOH	0.74	H_2O&H_2COO	0.46	H_2O&HCOOH	0.68	H_2O&CH_3O	0.59	H_2O&CH_2OH	0.65	H_2O&CH_3OH	0.67
CO&cis-COOH	0.74	CO&H_2COO	0.67	CO&HCOOH	0.69	CO&CH_3O	0.73	CO&CH_2OH	0.66	CO&CH_3OH	0.69
CO_2&cis-COOH	0.73	CO_2&H_2COO	0.59	CO_2&HCOOH	0.70	CO_2&CH_3O	0.68	CO_2&CH_2OH	0.71	CO_2&CH_3OH	0.70
CHO&cis-COOH	0.75	CHO&H_2COO	0.62	CHO&HCOOH	0.73	CHO&CH_3O	0.71	CHO&CH_2OH	0.69	CHO&CH_3OH	0.74
bi-HCOO&cis-COOH	0.66	bi-HCOO&H_2COO	0.45	bi-HCOO&HCOOH	0.67	bi-HCOO&CH_3O	0.50	bi-HCOO&CH_2OH	0.74	bi-HCOO&CH_3OH	0.62
mono-H_2CO&cis-COOH	0.73	mono-H_2CO&H_2COO	0.51	mono-H_2CO&HCOOH	0.64	mono-H_2CO&CH_3O	0.62	mono-H_2CO&CH_2OH	0.67	mono-H_2CO&CH_3OH	0.62
bi-H_2CO&cis-COOH	0.74	bi-H_2CO&H_2COO	0.59	bi-H_2CO&HCOOH	0.73	bi-H_2CO&CH_3O	0.69	bi-H_2CO&CH_2OH	0.71	bi-H_2CO&CH_3OH	0.74
trans-COOH&cis-COOH	0.74	trans-COOH&H_2COO	0.62	trans-COOH&HCOOH	0.73	trans-COOH&CH_3O	0.70	trans-COOH&CH_2OH	0.68	trans-COOH&CH_3OH	0.73
cis-COOH&cis-COOH	0.72	cis-COOH&H_2COO	0.55	cis-COOH&HCOOH	0.75	cis-COOH&CH_3O	0.64	cis-COOH&CH_2OH	0.72	cis-COOH&CH_3OH	0.74
H_2COO&cis-COOH	0.55	H_2COO&H_2COO	0.38	H_2COO&HCOOH	0.56	H_2COO&CH_3O	0.41	H_2COO&CH_2OH	0.59	H_2COO&CH_3OH	0.47
HCOOH&cis-COOH	0.75	HCOOH&H_2COO	0.56	HCOOH&HCOOH	0.68	HCOOH&CH_3O	0.69	HCOOH&CH_2OH	0.67	HCOOH&CH_3OH	0.69
CH_3O&cis-COOH	0.64	CH_3O&H_2COO	0.41	CH_3O&HCOOH	0.69	CH_3O&CH_3O	0.46	CH_3O&CH_2OH	0.69	CH_3O&CH_3OH	0.61

CH_2OH&cis-COOH	0.72	CH_2OH&H_2COO	0.59	CH_2OH&HCOOH	0.67	CH_2OH&CH_3O	0.69	CH_2OH&CH_2OH	0.61	CH_2OH&CH_3OH	0.65

Table S3. Summary of dual intermediate descriptors with an average determination coefficient of 0.75.

Main component	Paired components
bi-H_2CO	H_2O, CO_2, CHO, mono-H_2CO, trans-COOH, cis-COOH, CH_3OH
cis-COOH	H, H_2O, CO, bi-H_2CO, trans-COOH, CH_3OH
CHO	H_2O, CO_2, bi-H_2CO, CH_3OH
CO	O, bi-HCOO, cis-COOH
trans-COOH	CO_2, bi-H_2CO, cis-COOH
bi-HCOO	H_2, CO, CH_2OH
H_2O	CHO, bi-H_2CO, cis-COOH
CO_2	CHO, bi-H_2CO, trans-COOH
CH_3OH	CHO, bi-H_2CO, cis-COOH
H_2	O, bi-HCOO
O	CO
H	cis-COOH
CH_2OH	bi-HCOO
mono-H_2CO	bi-H_2CO

Table S4. Data statistics used in MLR for predicting thermodynamic properties research.

Substrate	***Species***	**DFT results**	EN_{IM}	Chg_{IM}	WF_{IM}	WF_{Sub}	SD_{Sub}	Chg_{IM-Sub}	BL_{IM-Sub}
Cu	*CO**	-247.03	5.99	10.26	8.961	4.398	0.13	0.26	1.97
	*CO_2**	-254.22	9.43	16.07	8.875	4.399	0.06	0.07	3.46
	*HCO**	-250.14	8.19	11.42	5.633	4.396	0.20	0.42	1.99
	*bi-HCOO**	-258.78	11.63	17.65	4.897	4.393	0.14	0.65	1.97
	*bi-H_2CO**	-254.19	10.39	12.75	6.187	4.395	0.27	0.75	2.10
	*trans-COOH**	-257.84	11.63	17.43	6.184	4.394	0.16	0.43	1.99
	*cis-COOH**	-257.93	11.63	17.49	6.794	4.395	0.21	0.49	1.99
	*H_2COO**	-262.16	13.83	19.10	7.441	4.393	0.24	1.10	1.96
	*HCOOH**	-261.40	13.83	18.01	6.664	4.397	0.11	0.01	2.13
	*CH_3O**	-258.47	12.59	13.57	6.031	4.395	0.16	0.57	1.96
	*CH_2OH**	-257.72	12.59	13.26	4.960	4.395	0.14	0.26	2.04
	*CH_3OH**	-262.00	14.79	14.01	6.165	4.398	0.10	0.01	2.11
	*(CO + H)**	-250.74	8.19	11.49	7.403	4.395	0.22	0.49	1.80
	*(CO + H_2O)**	-261.92	13.83	18.34	6.936	4.395	0.16	0.34	2.03
	*(CO_2 + H_C)**	-257.97	11.63	17.33	7.608	4.396	0.14	0.33	2.65
	*(CO_2 + H_O)**	-257.96	11.63	17.33	7.480	4.396	0.14	0.33	2.47
	*(HCO + H)**	-253.87	10.39	12.69	5.534	4.393	0.23	0.69	1.81
	*(HCO + OH)**	-261.25	13.83	19.08	6.478	4.394	0.38	1.08	2.03
	*(HCO + OH + H)**	-265.09	16.03	19.62	6.738	4.393	0.19	0.62	1.36
	*(bi-HCOO + H_C)**	-261.96	13.83	18.85	7.640	4.391	0.17	0.85	1.74
	*(bi-HCOO + H_O)**	-262.46	13.83	18.90	7.697	4.392	0.19	0.90	1.81
	*(bi-H_2CO + H_C)**	-257.85	12.59	13.99	6.197	4.394	0.31	0.99	1.88
	*(bi-H_2CO + H_O)**	-257.37	12.59	13.96	6.182	4.394	0.29	0.96	1.81
	*(bi-H_2CO+OH)**	-265.33	16.03	20.25	6.913	4.392	0.33	1.25	2.06

	*(bi-H_2CO+OH+H)**	-268.83	18.23	21.49	7.179	4.391	0.37	1.49	1.92
	*(bi-H_2CO+H_2O)**	-268.98	18.23	20.74	6.133	4.394	0.29	0.74	2.13
	*(trans-COOH+H)**	-261.55	13.83	18.69	6.194	4.392	0.21	0.69	1.82
	*(cis-COOH + H)**	-261.65	13.83	18.75	6.790	4.393	0.25	0.75	1.82
	*(H_2COO+H)**	-265.76	16.03	20.34	8.329	4.392	0.30	1.34	1.80
	*(HCOOH+H)**	-265.17	16.03	19.30	6.631	4.395	0.17	0.30	1.88
	*(CH_3O+H)**	-262.02	14.79	14.81	6.644	4.393	0.25	0.81	1.80
	*(CH_2OH+H)**	-261.38	14.79	14.52	4.972	4.394	0.20	0.52	1.85
	*CO**	-246.55	5.99	10.16	8.948	4.826	0.12	0.16	2.12
	*CO_2**	-254.01	9.43	16.06	8.901	4.825	0.04	0.06	3.66
	*HCO**	-249.60	8.19	11.15	5.285	4.824	0.07	0.15	1.95
	*bi-HCOO**	-258.15	11.63	17.62	7.528	4.815	0.21	0.62	1.96
	*bi-H_2CO**	-253.48	10.39	12.12	6.161	4.821	0.12	0.12	2.48
	*trans-COOH**	-257.23	11.63	17.24	6.008	4.824	0.15	0.24	2.09
	*cis-COOH**	-257.19	11.63	17.33	6.364	4.821	0.09	0.33	1.94
	*H_2COO**	-260.61	13.83	18.95	7.424	4.824	0.24	0.95	2.10
	*HCOOH**	-261.14	13.83	17.99	6.655	4.821	0.12	-0.01	2.14
Au-Cu	*CH_3O**	-257.66	12.59	13.54	6.168	4.820	0.39	0.54	2.01
	*CH_2OH**	-257.26	12.59	13.18	4.918	4.816	0.20	0.18	2.01
	*CH_3OH**	-261.73	14.79	13.99	6.132	4.822	0.11	-0.01	2.13
	*(CO + H)**	-250.07	8.19	11.26	7.513	4.823	0.14	0.26	1.78
	*(CO + H_2O)**	-261.30	13.83	18.18	7.148	4.822	0.16	0.18	2.11
	*(CO_2 + H_C)**	-257.53	11.63	17.20	7.563	4.826	0.11	0.20	2.70
	*(CO_2 + H_O)**	-257.51	11.63	17.19	7.515	4.826	0.10	0.19	2.72
	*(HCO + H)**	-253.10	10.39	12.30	5.126	4.825	0.13	0.30	1.83
	*(HCO + OH)**	-260.22	13.83	18.67	6.184	4.822	0.16	0.67	2.03
	*(HCO + OH + H)**	-263.89	16.03	19.55	6.751	4.823	0.14	0.55	2.44

	*(bi-HCOO + H_C)**	-261.63	13.83	18.76	7.479	4.816	0.23	0.76	1.84
	*(bi-HCOO + H_O)**	-261.63	13.83	18.76	7.613	4.816	0.23	0.76	1.84
	*(bi-H_2CO + H_C)**	-257.09	12.59	13.26	6.087	4.821	0.16	0.26	1.90
	*(bi-H_2CO + H_O)**	-256.97	12.59	13.22	6.165	4.821	0.14	0.22	1.91
	*(bi-H_2CO+OH)**	-264.66	16.03	19.54	19.304	4.817	0.17	0.54	1.98
	*(bi-H_2CO+OH+H)**	-268.15	18.23	20.69	7.119	4.817	0.20	0.69	1.85
	*(bi-H_2CO+H_2O)**	-268.12	18.23	20.02	5.778	4.820	0.13	0.02	2.53
	*(trans-COOH+H)**	-260.75	13.83	18.39	6.036	4.824	0.17	0.39	1.90
	*(cis-COOH + H)**	-260.96	13.83	18.56	6.727	4.818	0.25	0.56	1.86
	*(H_2COO+H)**	-264.10	16.03	20.08	7.474	4.826	0.27	1.08	1.91
	*(HCOOH+H)**	-264.66	16.03	19.17	6.622	4.821	0.16	0.17	1.92
	*(CH_3O+H)**	-261.14	14.79	14.68	6.161	4.820	0.41	0.68	1.86
	*(CH_2OH+H)**	-260.76	14.79	14.33	4.838	4.817	0.22	0.33	1.86
Ni-Cu	*CO**	-270.30	5.99	10.25	8.937	4.444	0.11	0.25	1.72
	*CO_2**	-277.38	9.43	16.61	8.412	4.441	0.19	0.61	1.98
	*HCO**	-273.28	8.19	11.62	5.719	4.443	0.31	0.62	1.89
	*bi-HCOO**	-281.58	11.63	17.65	7.793	4.443	0.18	0.65	1.89
	*bi-H_2CO**	-277.17	10.39	12.47	6.217	4.441	0.21	0.47	1.84
	*trans-COOH**	-280.97	11.63	17.45	6.389	4.443	0.21	0.45	1.88
	*cis-COOH**	-280.95	11.63	17.50	6.895	4.441	0.20	0.50	1.89
	*H_2COO**	-284.78	13.83	19.06	7.438	4.440	0.24	1.06	1.93
	*HCOOH**	-284.13	13.83	18.36	6.785	4.443	0.14	0.36	2.05
	*CH_3O**	-281.00	12.59	13.54	6.057	4.443	0.14	0.54	1.94
	*CH_2OH**	-280.48	12.59	13.24	5.089	4.444	0.20	0.24	1.99
	*CH_3OH**	-284.46	14.79	14.01	6.130	4.445	0.10	0.01	2.03
	*(CO + H)**	-274.19	8.19	11.49	7.487	4.445	0.14	0.49	1.68
	*(CO + H_2O)**	-285.39	13.83	18.27	7.041	4.442	0.15	0.27	1.89

	*(CO$_2$ + H_C)**	-281.26	11.63	17.85	7.595	4.440	0.22	0.85	1.80
	*(CO$_2$ + H_O)**	-281.26	11.63	17.85	7.503	4.438	0.22	0.85	1.80
	*(HCO + H)**	-278.00	10.39	12.66	5.734	4.443	0.20	0.66	1.74
	*(HCO + OH)**	-285.74	13.83	19.03	7.210	4.439	0.26	1.03	1.83
	*(HCO + OH + H)**	-289.43	16.03	20.24	7.144	4.438	0.30	1.24	1.79
	*(bi-HCOO + H_C)**	-285.50	13.83	18.90	7.610	4.442	0.21	0.90	1.75
	*(bi-HCOO + H_O)**	-285.50	13.83	18.90	7.629	4.441	0.21	0.90	1.75
	*(bi-H$_2$CO + H_C)**	-281.11	12.59	13.71	6.112	4.440	0.24	0.71	1.73
	*(bi-H$_2$CO + H_O)**	-281.07	12.59	13.71	6.175	4.440	0.24	0.71	1.73
	*(bi-H$_2$CO+OH)**	-288.34	16.03	20.09	7.034	4.443	0.43	1.09	1.98
	*(bi-H$_2$CO+OH+H)**	-292.02	18.23	21.15	6.585	4.442	0.40	1.15	1.83
	*(bi-H$_2$CO+H$_2$O)**	-291.97	18.23	20.48	5.816	4.444	0.23	0.48	2.03
	*(trans-COOH+H)**	-284.90	13.83	18.68	6.409	4.439	0.24	0.68	1.75
	*(cis-COOH + H)**	-284.87	13.83	18.74	6.055	4.436	0.23	0.74	1.75
	*(H$_2$COO+H)**	-288.75	16.03	20.30	7.415	4.436	0.27	1.30	1.78
	*(HCOOH+H)**	-288.06	16.03	19.60	7.255	4.442	0.17	0.60	1.84
	*(CH$_3$O+H)**	-284.98	14.79	14.79	5.929	4.442	0.18	0.79	1.78
	*(CH$_2$OH+H)**	-284.42	14.79	14.48	5.037	4.443	0.23	0.48	1.81
	*CO**	-278.97	5.99	10.20	8.960	4.414	0.38	0.20	2.05
	*CO$_2$**	-285.82	9.43	16.48	8.409	4.401	0.12	0.48	2.06
	*HCO**	-281.81	8.19	11.21	5.343	4.404	0.10	0.21	2.10
	*bi-HCOO**	-290.14	11.63	17.65	7.637	4.399	0.20	0.65	1.96
Pd-Cu	*bi-H$_2$CO**	-285.74	10.39	12.32	6.131	4.401	0.07	0.32	2.02
	*trans-COOH**	-289.41	11.63	17.29	6.096	4.405	0.12	0.29	2.04
	*cis-COOH**	-289.25	11.63	17.33	6.572	4.405	0.12	0.33	2.20
	*H$_2$COO**	-292.92	13.83	18.99	7.425	4.405	0.22	0.99	2.05
	*HCOOH**	-293.01	13.83	18.21	6.587	4.401	0.07	0.21	2.09

	*CH_3O**	-289.63	12.59	13.51	5.916	4.400	0.12	0.51	2.06
	*CH_2OH**	-289.29	12.59	13.07	4.663	4.406	0.11	0.07	2.09
	*CH_3OH**	-293.46	14.79	14.02	6.166	4.401	0.08	0.02	2.13
	*(CO + H)**	-282.71	8.19	11.37	7.480	4.419	0.39	0.37	1.86
	*(CO + H_2O)**	-293.73	13.83	18.18	7.026	4.414	0.39	0.18	2.22
	*(CO_2 + H_C)**	-289.62	11.63	17.51	8.072	4.405	0.16	0.51	1.91
	*(CO_2 + H_O)**	-289.62	11.63	17.51	8.118	4.405	0.16	0.51	1.92
	*(HCO + H)**	-285.58	10.39	12.37	5.396	4.407	0.14	0.37	1.90
	*(HCO + OH)**	-292.86	13.83	18.91	5.891	4.408	0.38	0.91	2.07
	*(HCO + OH + H)**	-296.41	16.03	19.77	6.765	4.402	0.23	0.77	2.14
	*(bi-HCOO + H_C)**	-293.90	13.83	18.82	7.576	4.403	0.22	0.82	1.82
	*(bi-HCOO + H_O)**	-293.90	13.83	18.82	7.518	4.403	0.22	0.82	1.82
	*(bi-H_2CO + H_C)**	-289.55	12.59	13.49	6.115	4.403	0.18	0.49	1.85
	*(bi-H_2CO + H_O)**	-289.54	12.59	13.49	6.128	4.405	0.12	0.49	1.85
	*(bi-H_2CO+OH)**	-296.65	16.03	19.80	6.679	4.399	0.22	0.80	2.12
	*(bi-H_2CO+OH+H)**	-300.17	18.23	20.93	6.672	4.405	0.24	0.93	1.96
	*(bi-H_2CO+H_2O)**	-300.60	18.23	20.32	5.955	4.401	0.10	0.32	2.09
	*(trans-COOH+H)**	-293.16	13.83	18.40	6.064	4.409	0.14	0.40	1.92
	*(cis-COOH + H)**	-293.01	13.83	18.43	6.597	4.411	0.16	0.43	2.00
	*(H_2COO+H)**	-296.72	16.03	20.15	7.392	4.408	0.24	1.15	1.86
	*(HCOOH+H)**	-296.75	16.03	19.41	6.584	4.403	0.15	0.41	1.91
	*(CH_3O+H)**	-293.46	14.79	14.68	5.984	4.404	0.15	0.68	1.87
	*(CH_2OH+H)**	-293.19	14.79	14.27	4.516	4.409	0.14	0.27	1.90
	*CO**	-294.36	5.99	10.19	9.011	4.894	0.38	0.19	2.04
	*CO_2**	-301.01	9.43	16.44	8.539	4.875	0.08	0.44	2.02
Pt-Cu	*HCO**	-297.14	8.19	11.06	5.055	4.898	0.10	0.06	1.96
	*bi-HCOO**	-304.90	11.63	17.61	7.627	4.856	0.21	0.61	1.94

*bi-H_2CO**	-300.90	10.39	12.33	6.129	4.872	0.08	0.33	2.00
*trans-COOH**	-304.90	11.63	17.22	6.043	4.867	0.13	0.22	2.00
*cis-COOH**	-304.53	11.63	17.22	6.362	4.882	0.09	0.22	1.98
*H_2COO**	-307.87	13.83	18.91	7.398	4.880	0.25	0.91	2.04
*HCOOH**	-308.07	13.83	18.25	6.566	4.873	0.08	0.25	2.05
*CH_3O**	-304.60	12.59	13.44	6.005	4.881	0.12	0.44	2.03
*CH_2OH**	-304.81	12.59	13.02	4.764	4.867	0.09	0.02	2.08
*CH_3OH**	-308.49	14.79	13.98	6.130	4.875	0.07	-0.03	2.08
*(CO + H)**	-298.36	8.19	11.30	7.478	4.891	0.38	0.30	1.87
*(CO + H_2O)**	-309.14	13.83	18.15	7.127	4.883	0.38	0.15	2.21
*(CO_2 + H_C)**	-304.79	11.63	17.45	7.527	4.881	0.13	0.45	1.80
*(CO_2 + H_O)**	-305.04	11.63	17.55	7.468	4.880	0.11	0.55	1.86
*(HCO + H)**	-301.17	10.39	12.18	5.025	4.888	0.13	0.18	1.83
*(HCO + OH)**	-307.92	13.83	18.62	4.459	4.884	0.25	0.62	2.07
*(HCO + OH + H)**	-311.84	16.03	19.13	7.022	4.877	0.10	0.13	1.93
*(bi-HCOO + H_C)**	-308.90	13.83	18.72	7.598	4.871	0.23	0.72	1.82
*(bi-HCOO + H_O)**	-308.90	13.83	18.72	7.597	4.870	0.22	0.72	1.82
*(bi-H_2CO + H_C)**	-304.18	12.59	13.48	6.088	4.876	0.12	0.48	1.71
*(bi-H_2CO + H_O)**	-304.93	12.59	13.45	6.093	4.880	0.11	0.45	1.85
*(bi-H_2CO+OH)**	-311.87	16.03	19.79	6.497	4.880	0.16	0.79	2.02
*(bi-H_2CO+OH+H)**	-315.78	18.23	20.88	6.936	4.885	0.19	0.88	1.92
*(bi-H_2CO+H_2O)**	-315.83	18.23	20.35	6.194	4.879	0.20	0.35	2.16
*(trans-COOH+H)**	-308.90	13.83	18.33	8.254	4.881	0.14	0.33	1.85
*(cis-COOH + H)**	-308.50	13.83	18.27	6.365	4.887	0.32	0.27	1.89
*(H_2COO+H)**	-311.91	16.03	20.03	7.289	4.884	0.27	1.03	1.87
*(HCOOH+H)**	-312.07	16.03	19.38	6.651	4.879	0.13	0.38	1.88
*(CH_3O+H)**	-308.63	14.79	14.56	6.065	4.867	0.14	0.56	1.87

	*(CH₂OH+H)**	-308.84	14.79	14.15	4.850	4.887	0.13	0.15	1.88
	*CO**	-211.41	5.99	10.19	8.978	4.479	0.52	0.19	1.84
	*CO_2**	-218.75	9.43	16.07	8.865	4.479	0.50	0.07	3.69
	*HCO**	-214.58	8.19	11.46	5.677	4.465	0.56	0.46	1.99
	*bi-HCOO**	-223.24	11.63	17.67	7.669	4.479	0.51	0.67	1.99
	*bi-H_2CO**	-218.43	10.39	12.79	6.191	4.478	0.60	0.79	2.16
	*trans-COOH**	-222.28	11.63	17.47	6.491	4.479	0.54	0.47	2.00
	*cis-COOH**	-222.33	11.63	17.51	6.757	4.448	0.53	0.51	2.00
	*H_2COO**	-226.58	13.83	19.16	7.442	4.479	0.57	1.16	1.98
	*HCOOH**	-225.80	13.83	18.03	6.602	4.466	0.50	0.03	2.28
	*CH_3O**	-222.97	12.59	13.60	6.102	4.479	0.54	0.60	1.98
	*CH_2OH**	-222.15	12.59	13.34	5.329	4.448	0.53	0.34	2.08
	*CH_3OH**	-226.44	14.79	14.02	6.127	4.468	0.50	0.02	2.19
	*(CO + H)**	-214.90	8.19	11.49	7.594	4.480	0.54	0.49	1.76
Zn-Cu	*(CO + H_2O)**	-226.14	13.83	18.22	7.113	4.479	0.52	0.22	2.05
	*(CO_2 + H_C)**	-222.27	11.63	17.37	7.565	4.479	0.52	0.37	2.69
	*(CO_2 + H_O)**	-222.26	11.63	17.36	7.602	4.479	0.52	0.36	2.73
	*(HCO + H)**	-218.09	10.39	12.76	5.627	4.464	0.58	0.76	1.84
	*(HCO + OH)**	-225.32	13.83	19.02	6.436	4.479	0.65	1.02	2.05
	*(HCO + OH + H)**	-229.48	16.03	19.65	6.747	4.479	0.55	0.65	2.07
	*(bi-HCOO + H_C)**	-226.76	13.83	18.95	7.496	4.479	0.54	0.95	1.84
	*(bi-HCOO + H_O)**	-226.70	13.83	18.95	7.663	4.448	0.54	0.95	1.84
	*(bi-H_2CO + H_C)**	-221.92	12.59	14.06	6.183	4.477	0.62	1.06	1.93
	*(bi-H_2CO + H_O)**	-221.51	12.59	14.02	6.217	4.478	0.62	1.02	1.84
	*(bi-H_2CO+OH)**	-229.66	16.03	20.31	6.190	4.478	0.63	1.31	2.09
	*(bi-H_2CO+OH+H)**	-232.94	18.23	21.57	6.930	4.478	0.67	1.57	1.96
	*(bi-H_2CO+H_2O)**	-233.18	18.23	20.82	5.998	4.477	0.62	0.82	2.19

*(trans-COOH+H)**	-225.51	13.83	18.80	6.244	4.478	0.56	0.80	1.80
*(cis-COOH + H)**	-225.82	13.83	18.79	6.741	4.478	0.56	0.79	1.84
*(H_2COO+H)**	-229.99	16.03	20.45	7.486	4.479	0.60	1.45	1.83
*(HCOOH+H)**	-229.34	16.03	19.33	6.615	4.464	0.53	0.33	1.96
*(CH_3O+H)**	-226.51	14.79	14.88	6.140	4.479	0.56	0.88	1.83
*(CH_2OH+H)**	-225.62	14.79	14.63	5.383	4.479	0.56	0.63	1.88

Table S5. Data statistics used in SISSO method for predicting thermodynamic properties research.

Substrate	***Species***	$SISSO_1$	$SISSO_2$	$SISSO_3$	$SISSO_4$	$SISSO_5$	$SISSO_6$	$SISSO_7$	$SISSO_8$
	*CO**	0.58	0.004	51.71	55.64	38.02	6.68	8.51	-268.52
	*CO_2**	0.84	0.001	80.23	87.15	66.94	11.76	15.16	-264.80
	*HCO**	0.65	0.009	44.15	48.12	38.38	6.74	8.53	-261.95
	*bi-H_2CO**	0.75	0.017	62.18	66.39	40.66	7.15	8.98	-259.94
	*trans-COOH**	0.61	0.006	69.93	73.91	38.41	6.75	8.58	-271.69
	*cis-COOH**	0.66	0.010	77.02	81.01	38.49	6.76	8.55	-271.37
	*CH_2OH**	0.61	0.005	60.40	64.49	39.43	6.93	8.83	-269.23
	*CH_3OH**	0.58	0.002	89.07	93.29	40.87	7.18	9.19	-280.12
	*(CO + H)**	0.63	0.011	58.83	62.43	34.85	6.13	7.71	-266.56
Cu	*(CO + H_2O)**	0.62	0.006	93.90	97.95	39.20	6.89	8.76	-279.30
	*(CO_2 + H_C)**	0.74	0.004	85.83	91.13	51.23	9.00	11.52	-271.64
	*(CO_2 + H_O)**	0.70	0.004	84.52	89.46	47.75	8.39	10.72	-273.02
	*(HCO + H)**	0.64	0.012	55.68	59.31	35.01	6.15	7.74	-263.93
	*(bi-H_2CO + H_C)**	0.73	0.021	76.14	79.90	36.32	6.39	7.96	-262.58
	*(bi-H_2CO + H_O)**	0.70	0.019	76.02	79.64	34.98	6.15	7.67	-264.82
	*(bi-H_2CO+H_2O)**	0.77	0.019	109.67	113.94	41.21	7.24	9.09	-272.86
	*(trans-COOH+H)**	0.62	0.010	83.85	87.48	35.03	6.16	7.77	-274.47
	*(cis-COOH + H)**	0.66	0.014	92.09	95.72	35.08	6.17	7.74	-274.27
	*(CH_2OH+H)**	0.62	0.009	71.69	75.38	35.62	6.26	7.91	-271.56
	*CO**	0.56	0.003	51.48	55.72	49.34	8.11	10.11	-255.14
	*CO_2**	0.80	0.000	80.28	87.60	85.21	14.00	17.62	-239.47
Au-Cu	*HCO**	0.47	0.001	41.33	45.23	45.38	7.46	9.34	-254.21
	*bi-H_2CO**	0.64	0.003	61.53	66.50	57.70	9.49	11.85	-248.82
	*trans-COOH**	0.58	0.005	67.78	71.97	48.72	8.01	9.95	-258.43

	*cis-COOH**	0.50	0.002	72.07	75.96	45.16	7.42	9.28	-262.30
	*CH_2OH**	0.62	0.009	59.91	63.92	46.53	7.65	9.46	-250.09
	*CH_3OH**	0.56	0.003	88.56	92.82	49.57	8.15	10.17	-264.45
	*(CO + H)**	0.51	0.004	59.75	63.31	41.41	6.81	8.44	-260.86
	*(CO + H_2O)**	0.60	0.006	96.75	100.97	49.07	8.07	10.01	-265.67
	*(CO_2 + H_C)**	0.67	0.003	85.26	90.66	62.85	10.33	12.91	-256.85
	*(CO_2 + H_O)**	0.67	0.002	84.68	90.12	63.41	10.42	13.03	-256.47
	*(HCO + H)**	0.51	0.004	51.43	55.09	42.61	7.00	8.70	-258.78
	*(bi-H_2CO + H_C)**	0.56	0.006	74.73	78.54	44.18	7.26	9.00	-261.65
	*(bi-H_2CO + H_O)**	0.53	0.004	75.71	79.53	44.40	7.30	9.07	-262.92
	*(bi-H_2CO+H_2O)**	0.66	0.004	102.81	107.86	58.69	9.65	12.04	-260.32
	*(trans-COOH+H)**	0.56	0.006	81.58	85.38	44.20	7.26	8.99	-265.30
	*(cis-COOH + H)**	0.64	0.013	91.18	94.89	43.15	7.10	8.71	-260.56
	*(CH_2OH+H)**	0.61	0.010	69.69	73.42	43.19	7.11	8.74	-255.21
	*CO**	0.50	0.003	51.82	55.25	33.91	5.91	7.52	-278.18
	*CO_2**	0.64	0.009	77.34	81.31	39.12	6.83	8.61	-280.56
	*HCO**	0.74	0.022	44.94	48.73	37.40	6.52	8.11	-260.16
	*bi-H_2CO**	0.62	0.010	62.76	66.43	36.24	6.32	7.95	-275.88
	*trans-COOH**	0.64	0.010	72.42	76.19	37.14	6.48	8.15	-278.35
	*cis-COOH**	0.63	0.009	78.30	82.07	37.19	6.49	8.17	-280.88
Ni-Cu	*CH_2OH**	0.64	0.009	62.08	66.06	39.22	6.84	8.63	-275.73
	*CH_3OH**	0.55	0.002	88.63	92.70	40.17	7.00	8.94	-288.35
	*(CO + H)**	0.52	0.005	59.64	62.99	33.10	5.77	7.30	-279.72
	*(CO + H_2O)**	0.58	0.005	95.49	99.27	37.26	6.50	8.23	-289.35
	*(CO_2 + H_C)**	0.63	0.011	86.53	90.13	35.53	6.20	7.78	-282.85
	*(CO_2 + H_O)**	0.63	0.011	85.46	89.06	35.51	6.20	7.78	-282.37
	*(HCO + H)**	0.60	0.009	57.84	61.31	34.26	5.98	7.51	-275.27

	*(bi-H_2CO + H_C)**	0.63	0.013	75.22	78.68	34.07	5.95	7.43	-277.88
	*(bi-H_2CO + H_O)**	0.63	0.013	76.01	79.47	34.12	5.95	7.44	-278.21
	*(bi-H_2CO+H_2O)**	0.69	0.012	103.99	108.06	40.13	7.00	8.80	-286.16
	*(trans-COOH+H)**	0.64	0.013	86.88	90.39	34.53	6.03	7.54	-281.34
	*(cis-COOH + H)**	0.63	0.012	81.99	85.50	34.53	6.03	7.55	-280.27
	*(CH_2OH+H)**	0.63	0.012	72.69	76.30	35.67	6.22	7.80	-277.97
	*CO**	0.84	0.033	51.62	55.72	39.86	6.99	8.65	-248.37
	*CO_2**	0.59	0.003	77.24	81.36	39.93	7.01	8.95	-277.06
	*HCO**	0.58	0.002	41.66	45.86	40.73	7.15	9.15	-266.61
	*bi-H_2CO**	0.53	0.001	61.68	65.72	39.17	6.88	8.83	-273.51
	*trans-COOH**	0.58	0.003	68.86	72.93	39.51	6.93	8.85	-275.67
	*cis-COOH**	0.62	0.003	74.24	78.63	42.59	7.47	9.55	-276.06
	*CH_2OH**	0.58	0.003	56.61	60.80	40.62	7.13	9.11	-271.87
	*CH_3OH**	0.57	0.002	89.07	93.32	41.24	7.24	9.29	-281.19
	*(CO + H)**	0.82	0.035	59.40	63.13	36.40	6.37	7.84	-250.90
Pd-Cu	*(CO + H_2O)**	0.89	0.034	94.95	99.39	43.23	7.58	9.41	-259.29
	*(CO_2 + H_C)**	0.60	0.006	91.96	95.79	37.15	6.52	8.27	-282.48
	*(CO_2 + H_O)**	0.60	0.006	92.50	96.33	37.16	6.52	8.27	-282.58
	*(HCO + H)**	0.57	0.004	54.16	57.97	36.92	6.48	8.24	-272.10
	*(bi-H_2CO + H_C)**	0.60	0.008	75.14	78.84	35.88	6.30	7.97	-275.99
	*(bi-H_2CO + H_O)**	0.54	0.003	75.30	79.00	35.91	6.30	8.03	-279.51
	*(bi-H_2CO+H_2O)**	0.58	0.002	106.47	110.65	40.53	7.12	9.10	-286.68
	*(trans-COOH+H)**	0.58	0.005	81.95	85.78	37.29	6.54	8.32	-281.06
	*(cis-COOH + H)**	0.61	0.005	89.24	93.23	38.87	6.81	8.66	-282.59
	*(CH_2OH+H)**	0.57	0.005	64.89	68.69	36.95	6.48	8.24	-275.80
Pt-Cu	*CO**	0.80	0.029	51.93	56.02	48.93	7.96	9.62	-294.73
	*CO_2**	0.50	0.001	78.51	82.54	47.95	7.82	9.75	-304.58

	*HCO**	0.50	0.002	39.44	43.36	47.00	7.64	9.49	-315.44
	*bi-H_2CO**	0.49	0.001	61.68	65.68	47.54	7.76	9.68	-296.24
	*trans-COOH**	0.54	0.003	68.28	72.28	47.46	7.75	9.63	-292.84
	*cis-COOH**	0.50	0.002	72.01	75.97	47.29	7.70	9.59	-309.19
	*CH_2OH**	0.52	0.002	57.90	62.06	49.22	8.04	10.02	-290.18
	*CH_3OH**	0.50	0.001	88.58	92.75	49.50	8.07	10.09	-308.15
	*(CO + H)**	0.77	0.030	59.37	63.12	44.78	7.28	8.77	-291.20
	*(CO + H_2O)**	0.84	0.030	96.35	100.78	52.73	8.59	10.41	-297.32
	*(CO_2 + H_C)**	0.50	0.004	85.74	89.34	42.94	7.00	8.66	-310.50
	*(CO_2 + H_O)**	0.49	0.002	85.00	88.71	44.24	7.21	8.96	-310.29
	*(HCO + H)**	0.50	0.003	50.38	54.04	43.78	7.12	8.83	-306.14
	*(bi-H_2CO + H_C)**	0.47	0.003	74.94	78.36	40.69	6.63	8.22	-302.53
	*(bi-H_2CO + H_O)**	0.49	0.002	74.86	78.56	44.04	7.18	8.91	-306.98
	*(bi-H_2CO+H_2O)**	0.65	0.009	110.76	115.08	51.44	8.38	10.34	-315.15
	*(trans-COOH+H)**	0.52	0.004	112.30	116.00	44.10	7.18	8.89	-319.00
	*(cis-COOH + H)**	0.71	0.022	86.14	89.92	45.19	7.35	8.92	-303.30
	*(CH_2OH+H)**	0.52	0.003	69.85	73.62	45.00	7.32	9.08	-311.85
	*CO**	0.93	0.060	51.94	55.62	36.93	6.40	7.73	-227.95
	*CO_2**	1.32	0.055	79.91	87.28	73.94	12.82	16.01	-228.02
	*HCO**	1.00	0.070	44.51	48.48	39.62	6.89	8.32	-216.47
	*bi-H_2CO**	1.09	0.081	62.16	66.48	43.31	7.51	9.07	-209.14
	*trans-COOH**	0.98	0.064	73.49	77.49	40.18	6.97	8.44	-229.77
Zn-Cu	*cis-COOH**	0.98	0.064	76.58	80.59	39.64	6.91	8.38	-232.26
	*CH_2OH**	1.00	0.064	65.01	69.17	41.19	7.18	8.73	-227.79
	*CH_3OH**	0.99	0.057	88.43	92.81	43.74	7.60	9.29	-240.75
	*(CO + H)**	0.93	0.065	60.43	63.96	35.39	6.14	7.36	-225.99
	*(CO + H_2O)**	0.98	0.060	96.32	100.42	41.11	7.13	8.66	-240.03

*(CO_2 + H_C)**	1.12	0.061	85.29	90.67	54.02	9.37	11.54	-231.23
*(CO_2 + H_O)**	1.13	0.061	85.68	91.15	54.85	9.51	11.72	-231.35
*(HCO + H)**	0.99	0.074	56.63	60.30	36.61	6.36	7.63	-216.98
*(bi-H_2CO + H_C)**	1.05	0.086	75.91	79.77	38.67	6.71	8.02	-210.51
*(bi-H_2CO + H_O)**	1.03	0.087	76.43	80.11	36.94	6.41	7.62	-210.79
*(bi-H_2CO+H_2O)**	1.11	0.087	107.16	111.53	43.81	7.60	9.16	-218.57
*(trans-COOH+H)**	0.96	0.069	84.56	88.15	36.03	6.25	7.49	-229.96
*(cis-COOH + H)**	0.97	0.070	91.38	95.07	36.98	6.41	7.70	-231.11
*(CH_2OH+H)**	0.98	0.069	77.73	81.50	37.75	6.55	7.87	-227.31

Table S6. Linear performance (PCC) of CO&O and CHO&CH_3OH descriptors in the data of [29].

Intermediate	CO&O	CHO&CH_3OH
H	0.988	0.997
CO	0.948	0.967
CO_2	0.991	0.994
O	0.989	0.972
OH	0.857	0.861
H_2O	0.986	0.979
CHO	0.995	0.997
CH_2O	0.745	0.741
CH_3O	0.328	0.387
CH_3OH	0.959	0.977

Table S7. Linear performance (PCC) of CO&O and CHO&CH_3OH descriptors in the data of [64].

Intermediate	CO&O	CHO&CH_3OH
H	0.906	0.927
O	0.971	0.982
C	0.992	0.997
CO_2	0.998	1.000
H_2O	0.964	0.977
COOH	0.999	1.000
HCOO	0.987	0.994
HCOOH	0.985	0.993
CH_2OH	0.993	0.998
H_2COOH	0.991	0.996
CH_3OH	0.957	0.971