Supplementary Information

Molecular understanding of the impacts of structural characteristics on ethanol adsorption performance for adsorption heat pumps

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Supplementary Information (SI) includes:

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Table S1. The tunable parameters of pseudo material in this work.

Parameter	Cell length *l* (Å)	σ (Å)	ε (kJ/mol)
Range	5-35	1-6	0.042-4.2
Presetting value	5, 7.5, 10, 12.5, 15, 17.5, 20, 22.5, 25, 27.5, 30, 32.5, 35	1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8, 5.0, 5.2, 5.4, 5.6, 5.8, 6.0	0.042, 0.084, 0.168, 0.252, 0.336, 0.42, 0.84, 1.68, 2.52, 3.36, 4.2

Table S2. TraPPE force field parameters of ethanol.

adsorbate	interaction site	σ (Å)	ε/k_B (kJ/mol)	*q* (e)
ethanol	CH_3	3.75	0.819	0
	CH_2	3.95	0.3822	0.265
	O	3.02	0.777	-0.7
	H	0	0	0.435

Table S3. The uptake and uptake change ($dW=W_{i+1} - W_i$) of structure with σ = 1 Å, ε = 0.252, 0.336, 2.52, and 3.36 kJ/mol, which the maximum $dW(W_\alpha)$ were highlighted in green.

P/P_0		0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
ε=0.252	W (mg/g)	0.0009	0.0025	0.0027	0.0042	0.0044	0.0064	0.0069	0.0076	0.0088	0.0105
	dW (mg/g)	0.0009	0.0016	0.0002	0.0015	0.0002	0.002	0.0005	0.0007	0.0012	0.0017
ε=0.336	W (mg/g)	0.0015	0.0031	0.004	0.0058	0.0068	0.0088	0.009	0.0114	0.0122	0.0141
	dW (mg/g)	0.0015	0.0016	0.0009	0.0018	0.001	0.002	0.0002	0.0024	0.0008	0.0019
ε=2.52	W (mg/g)	0.07	0.13	0.22	0.28	0.34	0.41	0.56	9.94	13.68	287.23
	dW (mg/g)	0.07	0.06	0.09	0.06	0.06	0.07	0.15	9.38	3.74	277.29
ε=3.36	W (mg/g)	0.39	1.58	287.83	287.74	287.94	288.14	288.16	288.17	288.16	288.2
	dW (mg/g)	0.39	1.19	286.25	-0.09	0.2	0.2	0.02	0.01	-0.01	0.04

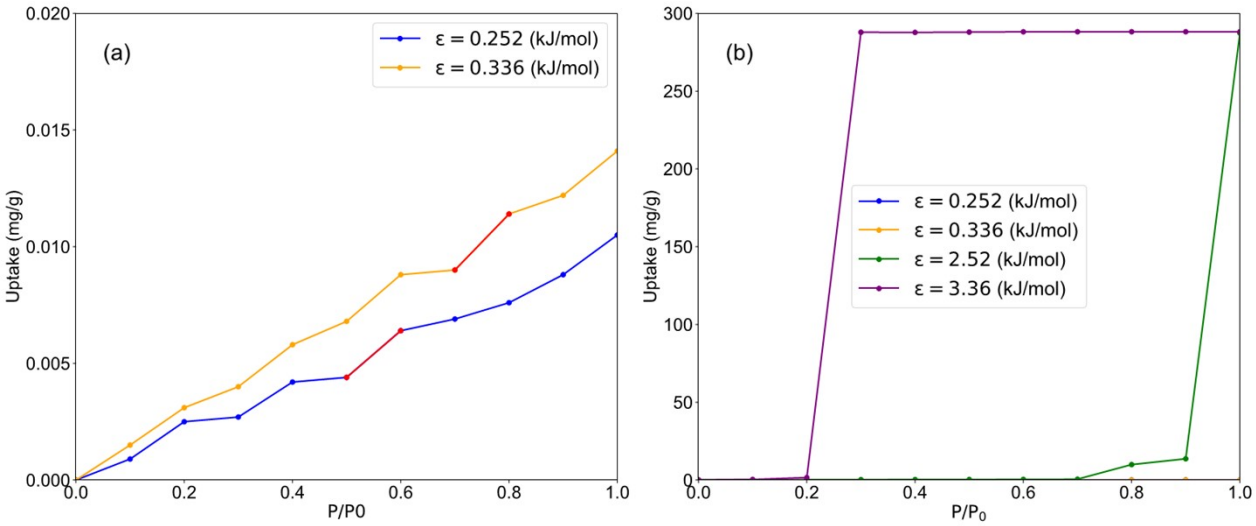

Figure S1. (a) The adsorption isotherm of structures with σ = 1 Å, ε = 0.252, 0.336 kJ/mol, the step location was colored in red. (b) The adsorption isotherm of structures with σ = 1 Å, ε = 0.252, 0.336, 2.52, 3.36 kJ/mol.

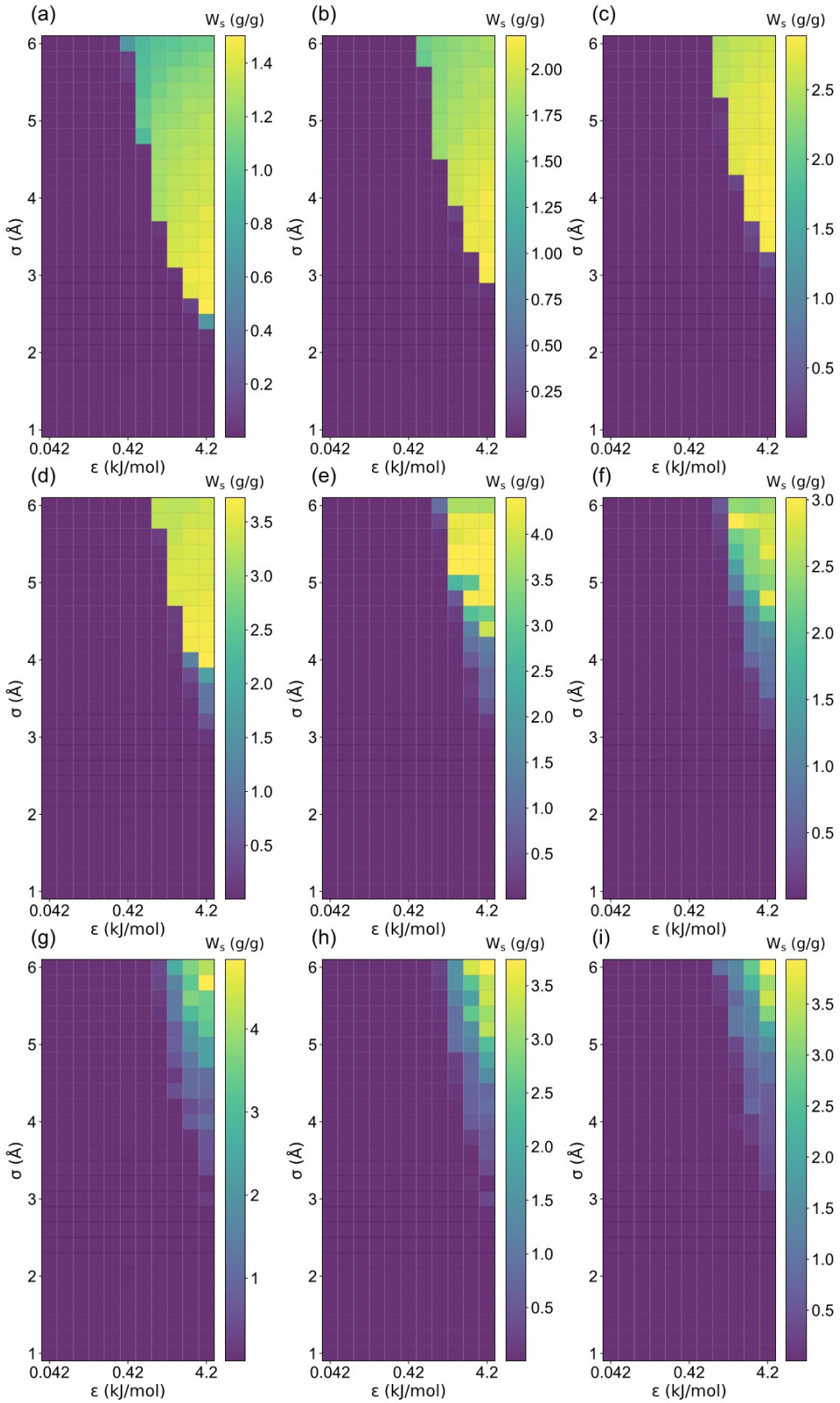

Figure S2. The saturation capacity (W_s) changed with σ and ε in (a) *l* = 12.5 , (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure.

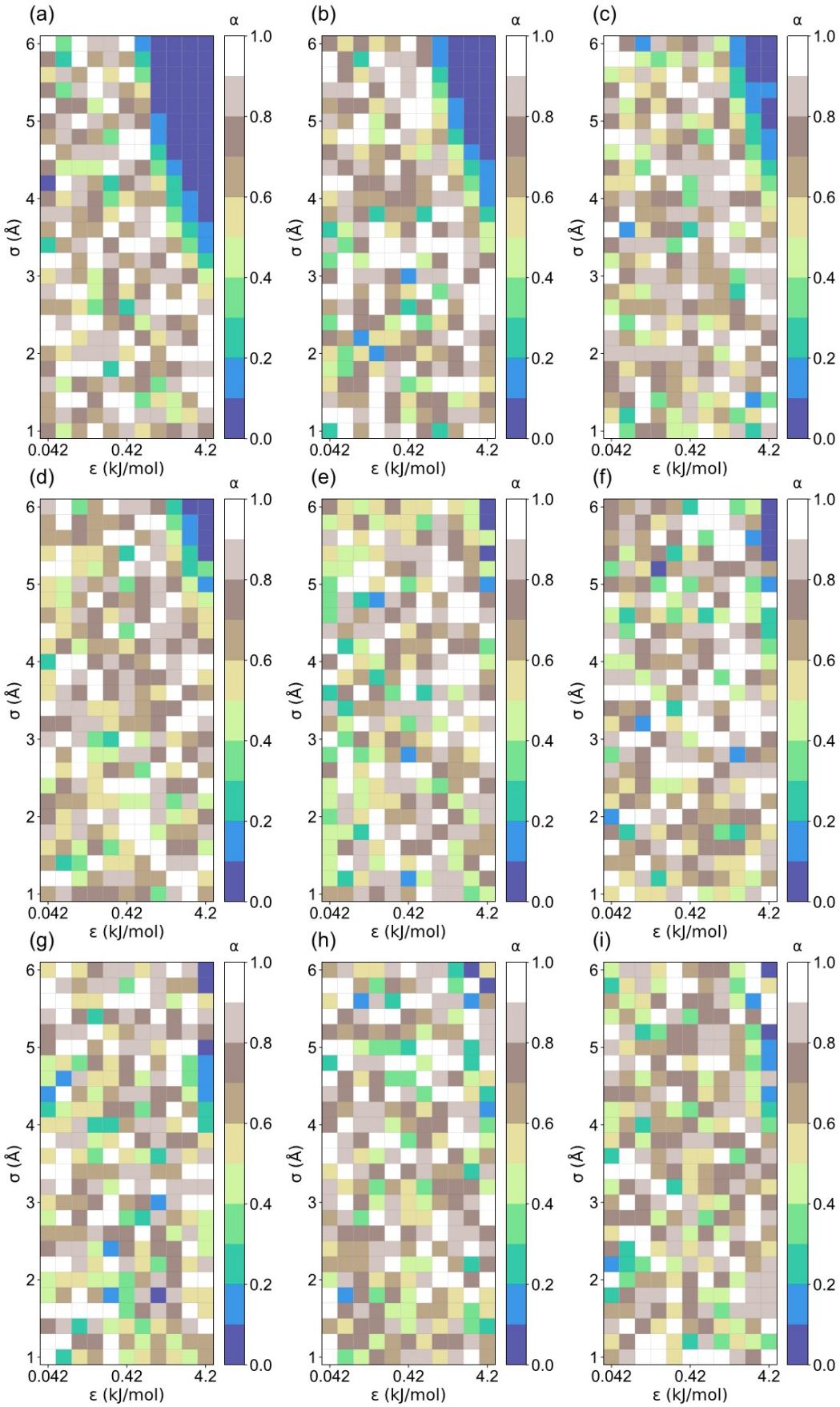

Figure S3. The step location (α) changed with σ and ε in (a) *l* = 12.5 , (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure.

Table S4. The ratio of maximum W_α compared to W_s for a fixed cell length.

l	5 Å	7.5 Å	10 Å	12.5 Å	15 Å	17.5 Å	20 Å
W_α/W_s	0.99	0.94	0.94	0.90	0.85	0.87	0.77
l	22.5 Å	25 Å	27.5 Å	30 Å	32.5 Å	35 Å	
W_α/W_s	0.55	0.29	0.25	0.34	0.22	0.25	

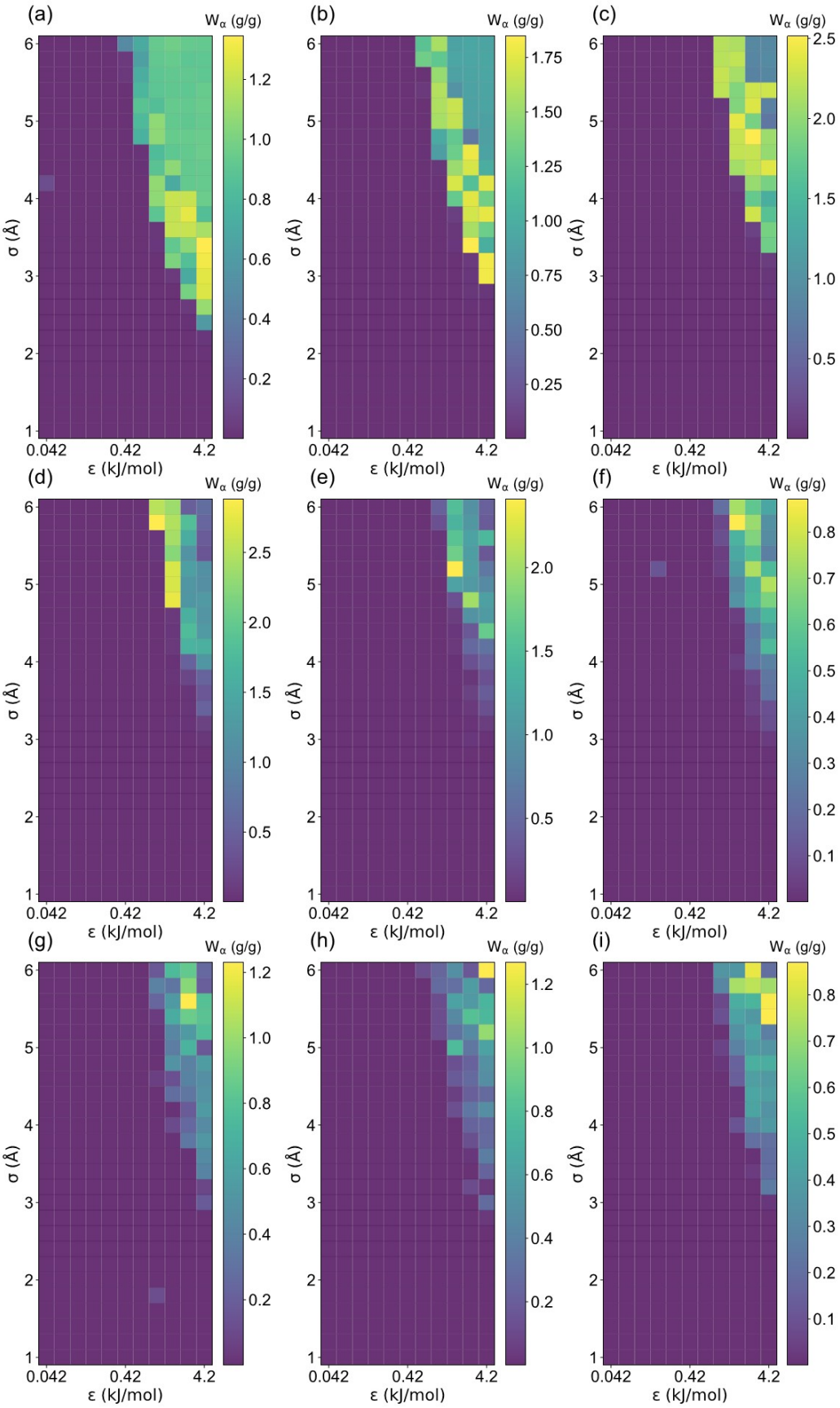

Figure S4. The uptake change at step location (W_α) changed with σ and ε in (a) *l* = 12.5 , (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure.

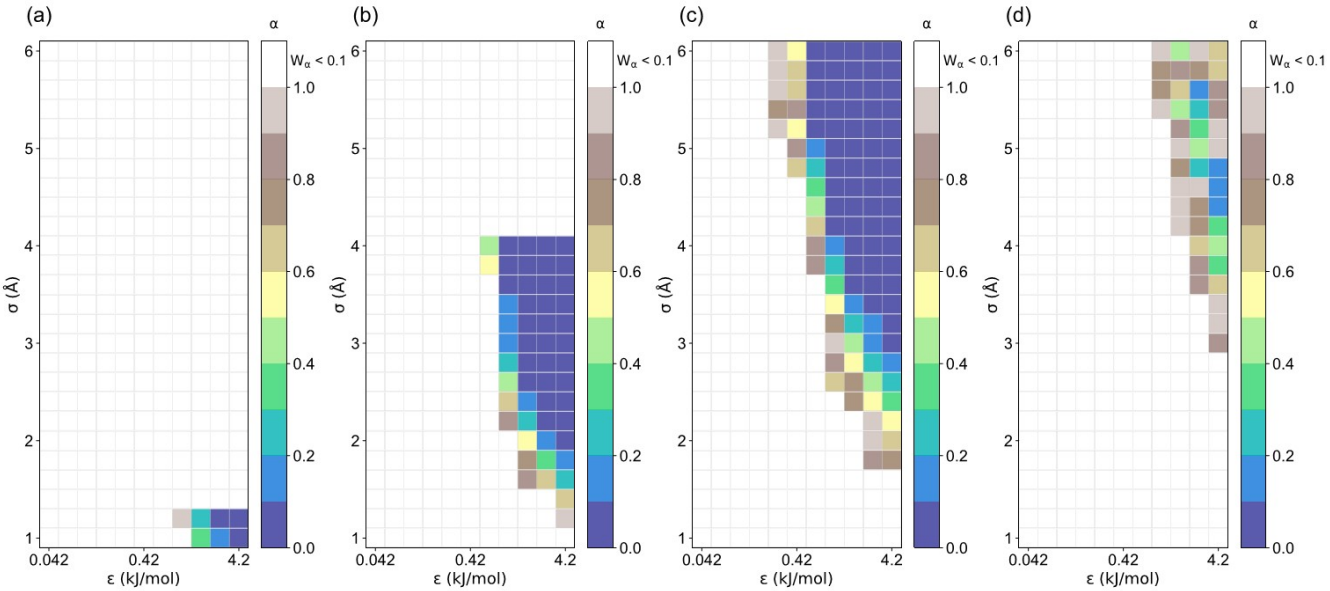

Figure S5. The step location (α) changed with σ and ε in (a) *l* = 5 , (b) *l* = 7.5, (c) *l* = 10 and (d) *l* = 35 Å structure, which step location with $W_α$ < 0.01 g/g were colored by white.

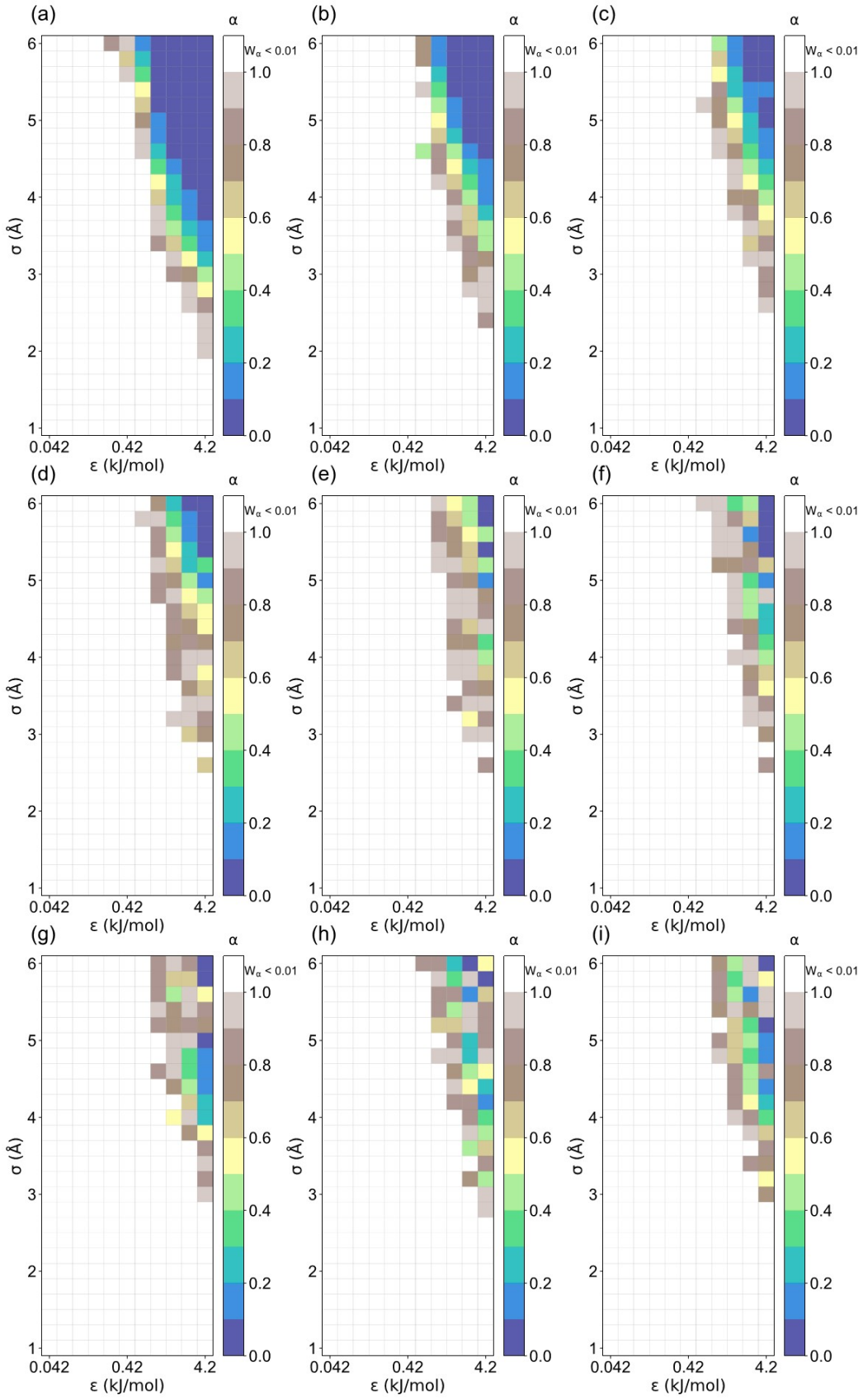

Figure S6. The step location (α) changed with σ and ε in (a) *l* = 12.5 , (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure, which step location with $W_\alpha < 0.01$ g/g were colored by white.

Table S5. The percentage of $W_\alpha > 0.1$ g/g structures for fixed *l*.

l	5 Å	7.5 Å	10 Å	12.5 Å	15 Å	17.5 Å	20 Å
Ratio	2.4%	18.5%	36.7%	28.3%	22.4%	18.9%	18.9%
l	22.5 Å	25 Å	27.5 Å	30 Å	32.5 Å	35 Å	
Ratio	17.8%	16.8%	15.4%	16.1%	0.22	15%	

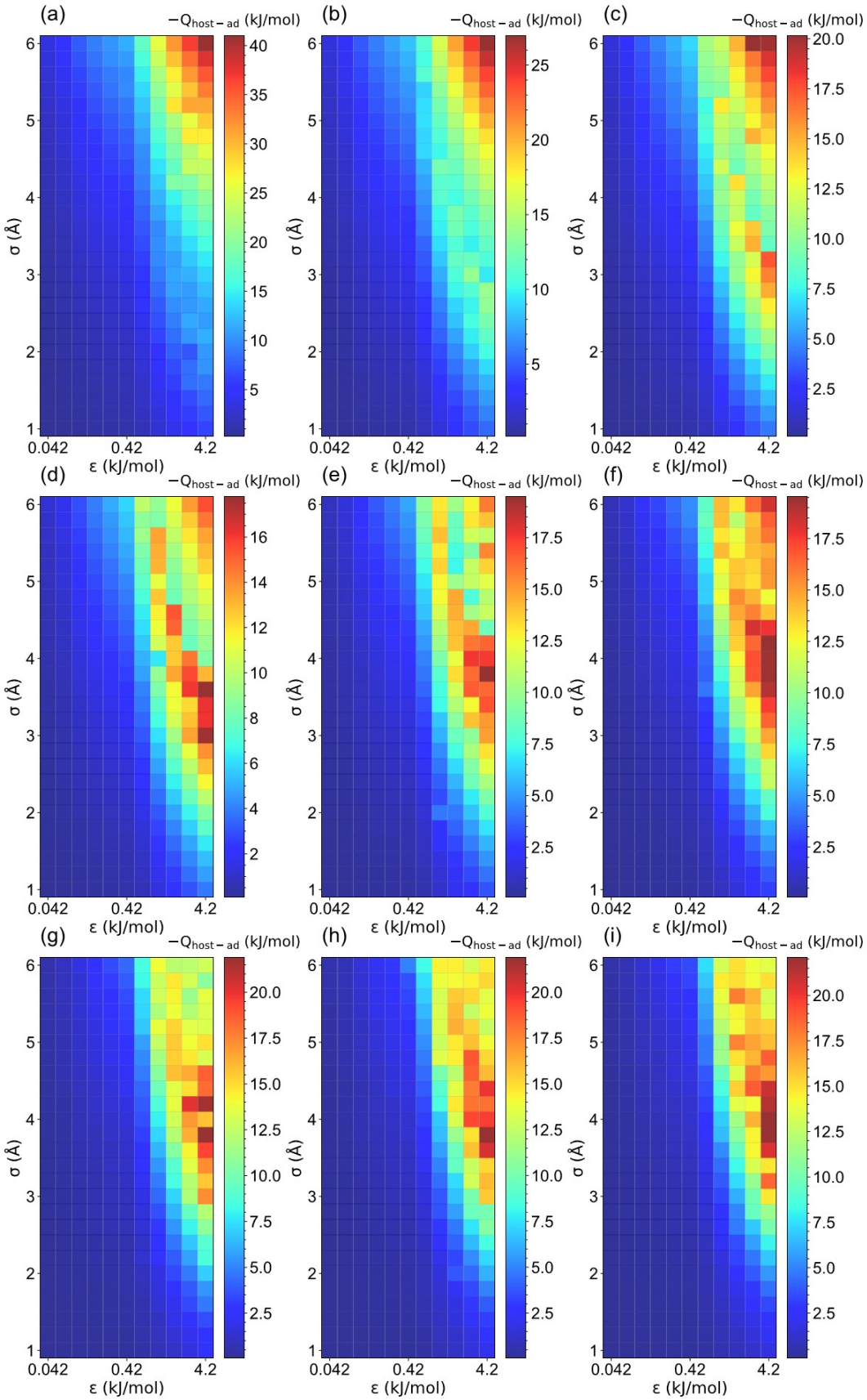

Figure S7. The host-adsorbate interaction ($Q_{host-ad}$) changed with σ and ε in (a) *l* = 12.5 , (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure.

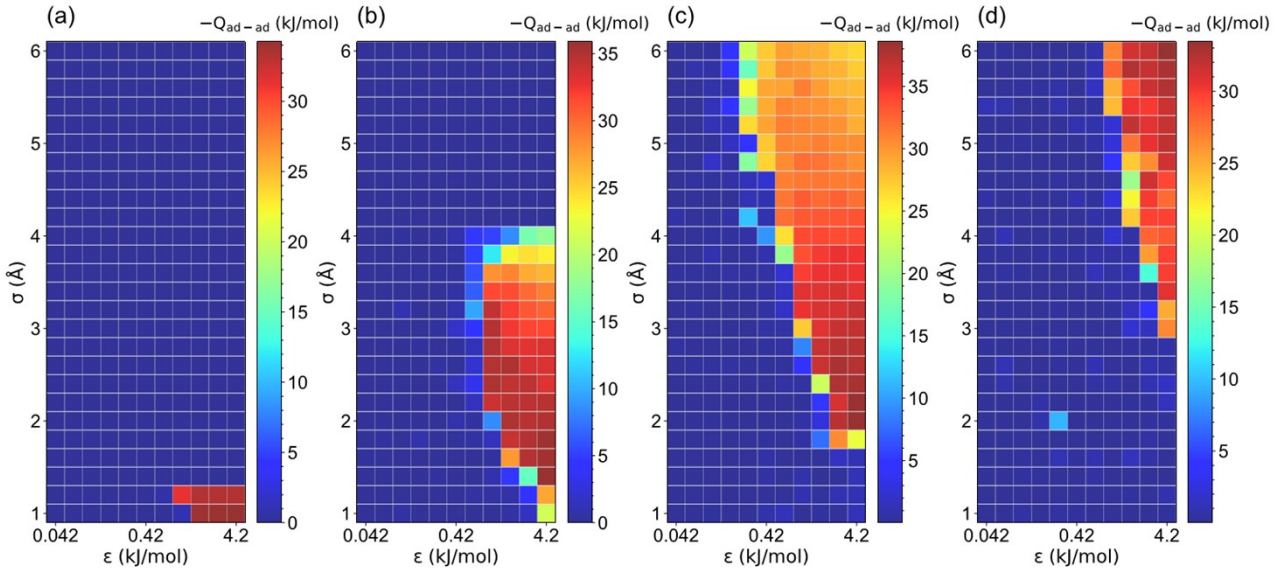

Figure S8. The adsorbate-adsorbate interaction (Q_{ad-ad}) of ethanol under various LJ parameter (σ and ε) in (a) *l* = 5, (b) *l* = 7.5, (c) *l* = 10 and (d) *l* = 35 Å structure.

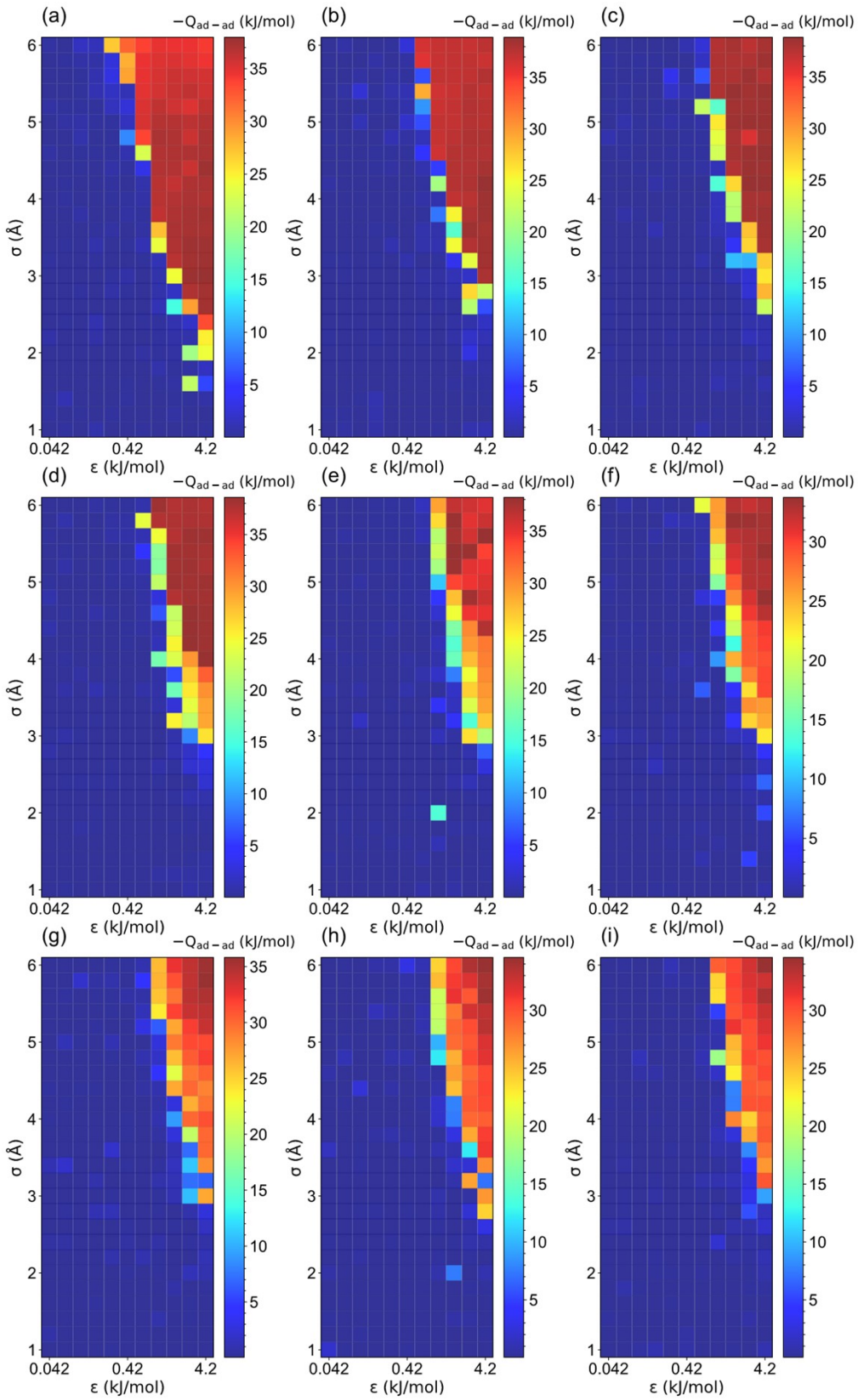

Figure S9. The adsorbate-adsorbate interaction ($Q_{ad\text{-}ad}$) of ethanol under various LJ parameter (σ and ε) in (a) *l* = 12.5, (b) *l* = 15, (c) *l* = 17.5, (d) *l* = 20, (e) *l* = 22.5, (f) *l* = 25, (g) *l* = 27.5, (h) *l* = 30 and (i) *l* = 32.5 Å structure.