Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION:

Cross-impact of surface and interaction anisotropy in the self-assembly of organic adsorption monolayers: Monte Carlo and transfer-matrix study

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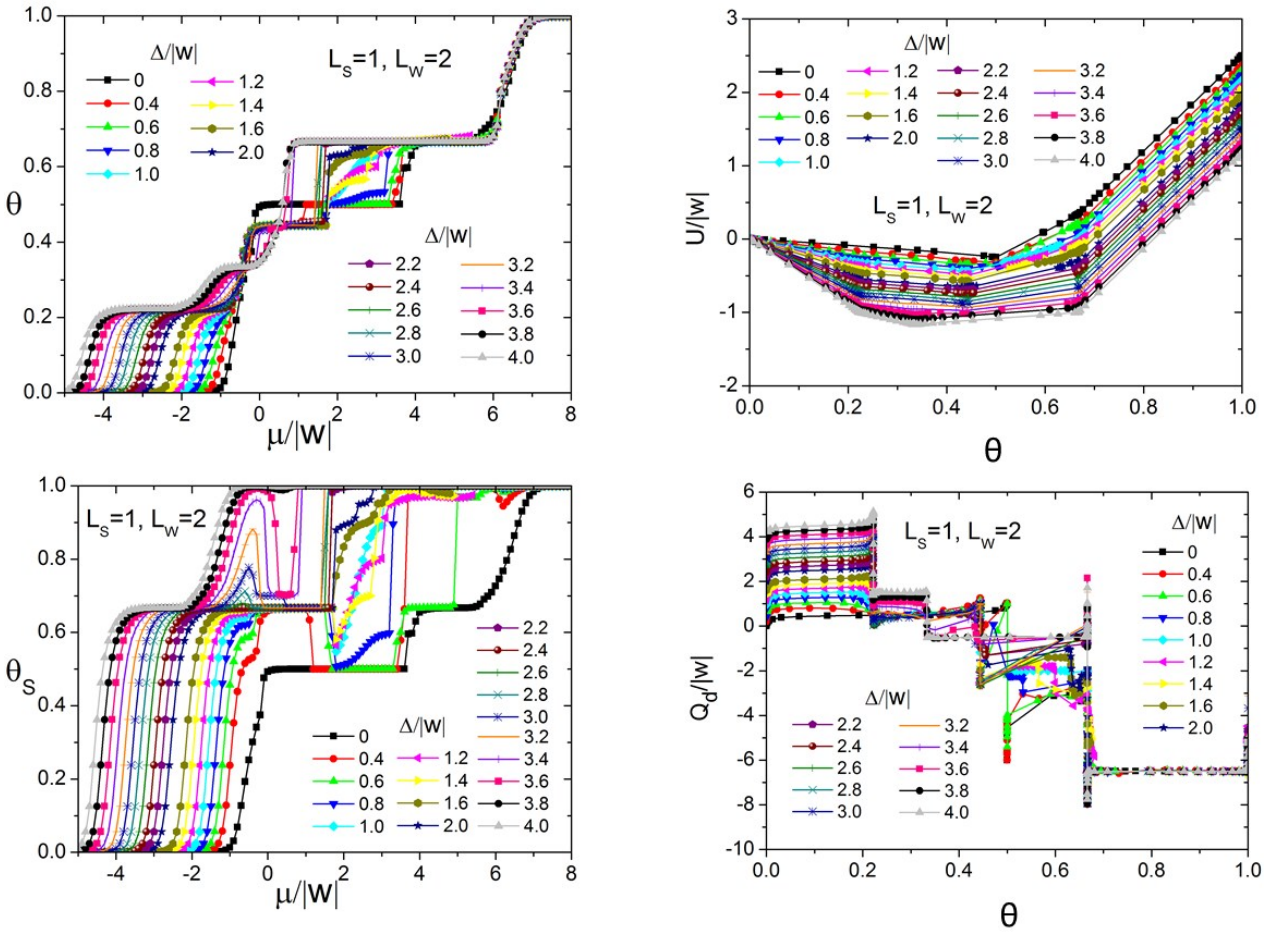


Fig. S1 Total adsorption isotherms – θ(μ/|w|), partial adsorption isotherms for the "strong" sites – $\theta_S(\mu/|w|)$, internal energy and differential heat of adsorption vs. surface coverage – U(θ) and $Q_d(\theta)$, correspondingly. All curves were calculated for the surface with $L_s=1$ and $L_w=2$ topography at ε/|w|=2, RT/|w|=0.1662.

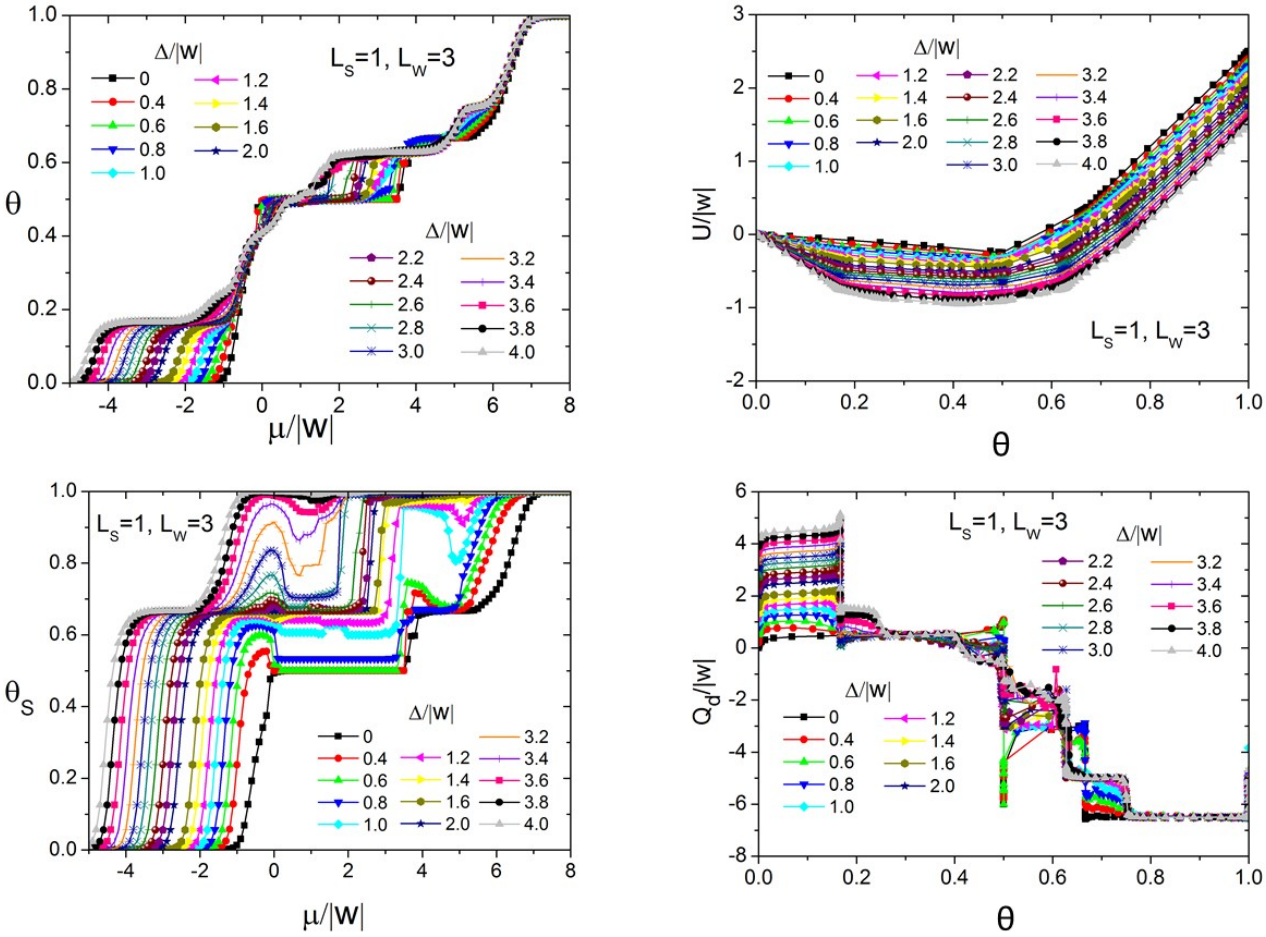


Fig. S2 Total adsorption isotherms – $\theta(\mu/|w|)$, partial adsorption isotherms for the "strong" sites – $\theta_S(\mu/|w|)$, internal energy and differential heat of adsorption vs. surface coverage – $U(\theta)$ and $Q_d(\theta)$, correspondingly. All curves were calculated for the surface with $L_s=1$ and $L_w=3$ topography $\varepsilon/|w|=2$, $RT/|w|=0.1662$.

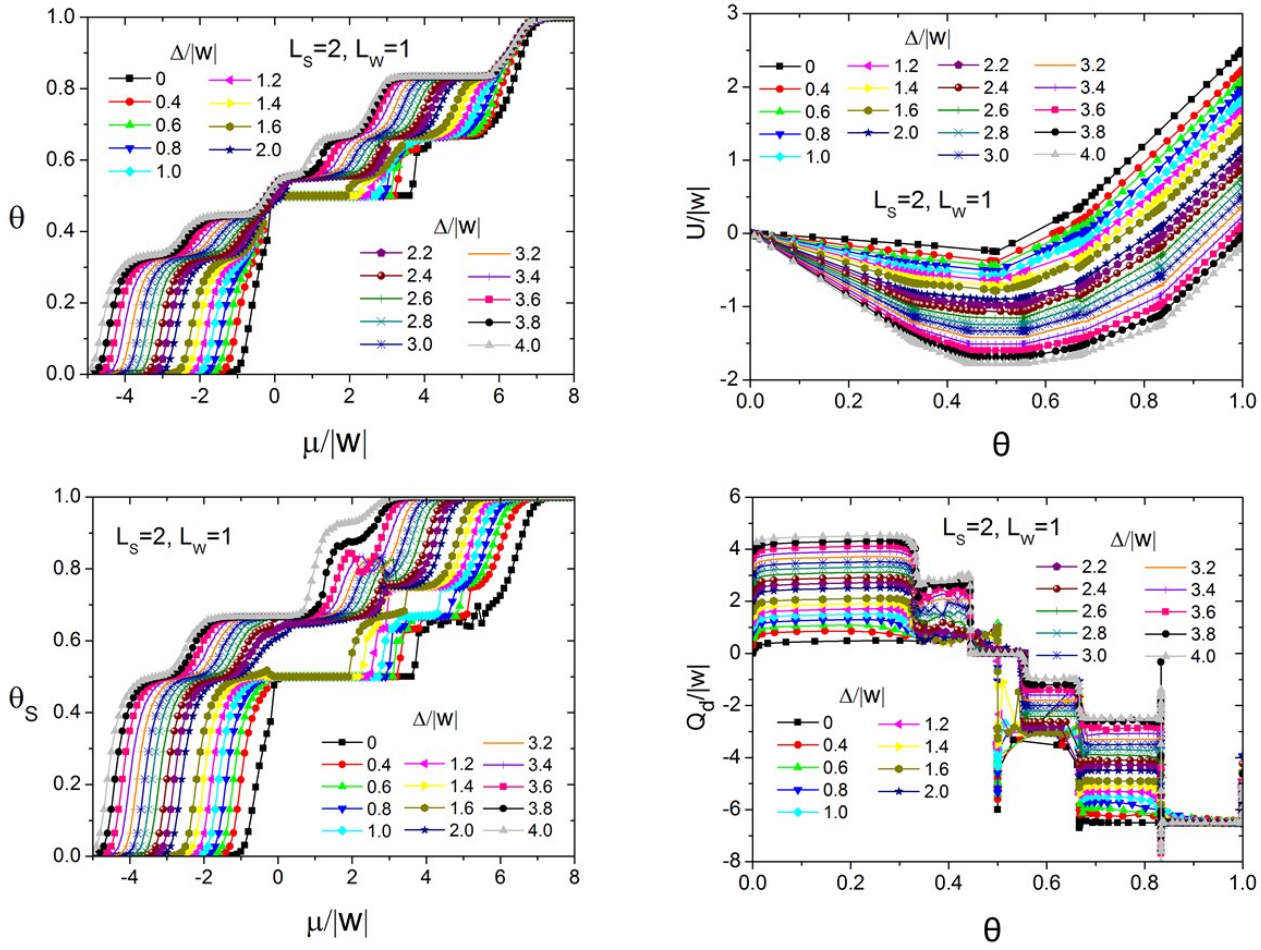


Fig. S3 Total adsorption isotherms – θ(μ/|w|), partial adsorption isotherms for the "strong" sites – θ_S(μ/|w|), internal energy and differential heat of adsorption vs. surface coverage – U(θ) and Q_d(θ), correspondingly. All curves were calculated for the surface with L_s=*2* and L_w=*1* topography ε/|w|=2, RT/|w|=0.1662.

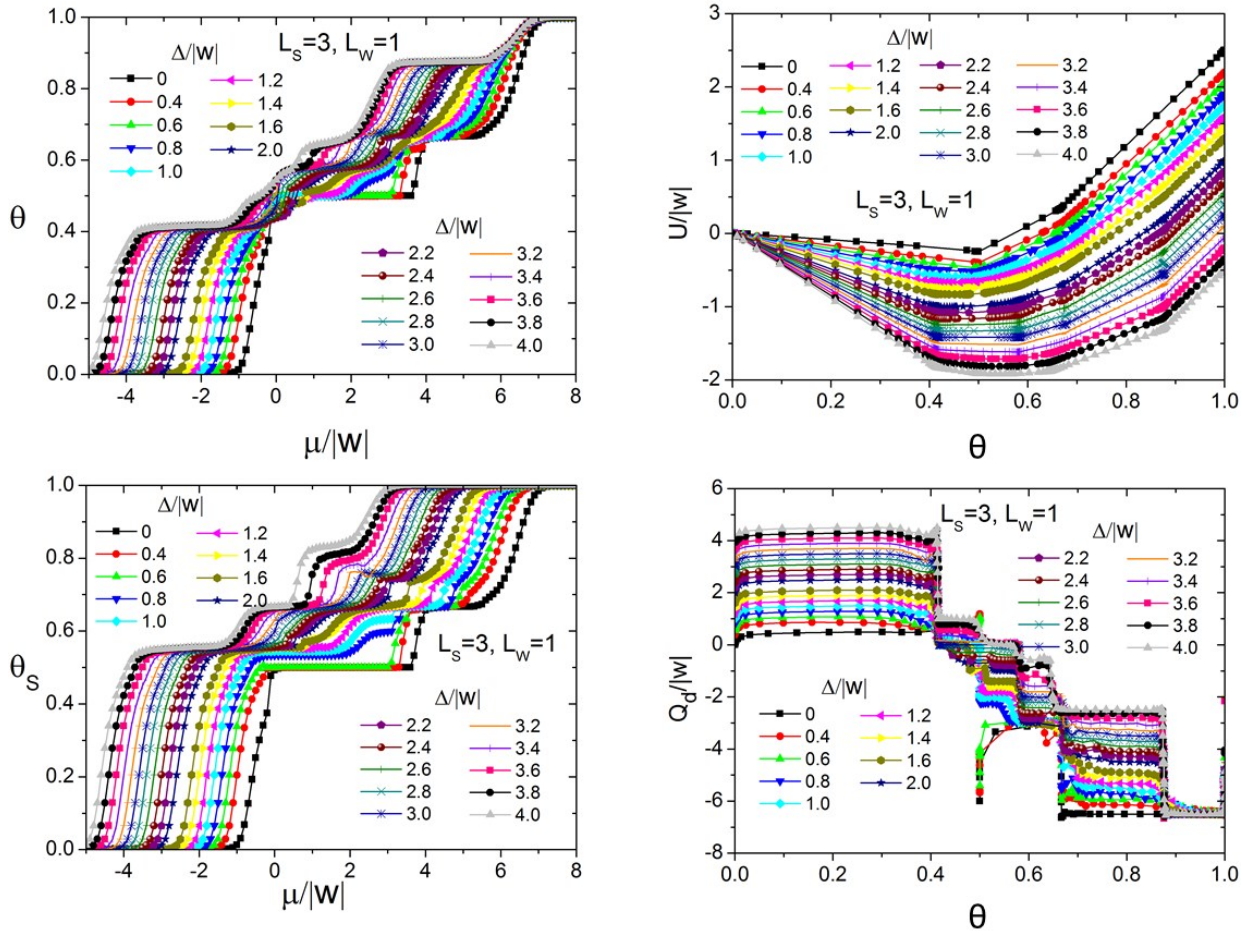
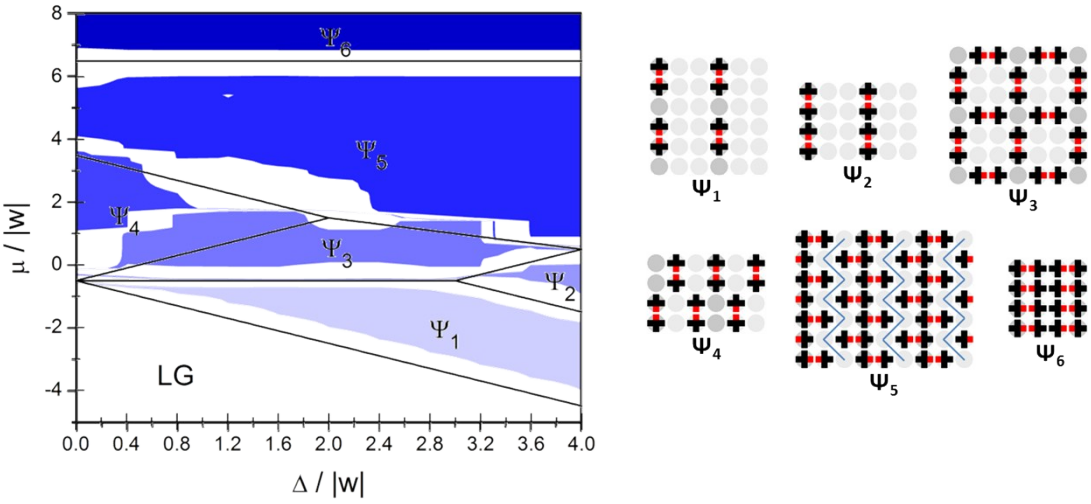
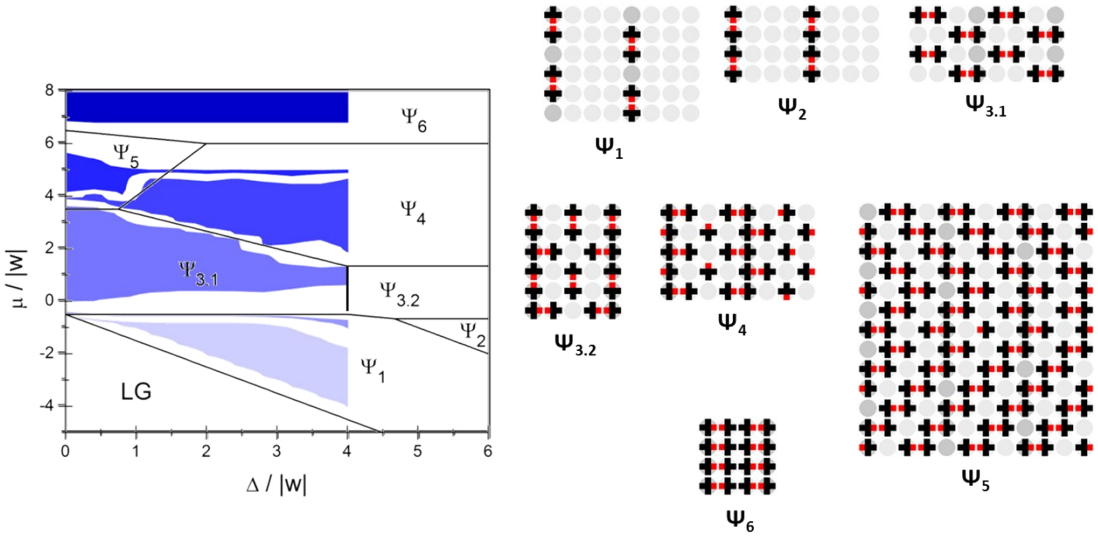


Fig. S4 Total adsorption isotherms – $\theta(\mu/|w|)$, partial adsorption isotherms for the "strong" sites – $\theta_S(\mu/|w|)$, internal energy and differential heat of adsorption vs. surface coverage – $U(\theta)$ and $Q_d(\theta)$, correspondingly. All curves were calculated for the surface with $L_s=3$ and $L_w=1$ topography $\varepsilon/|w|=2$, $RT/|w|=0.1662$.



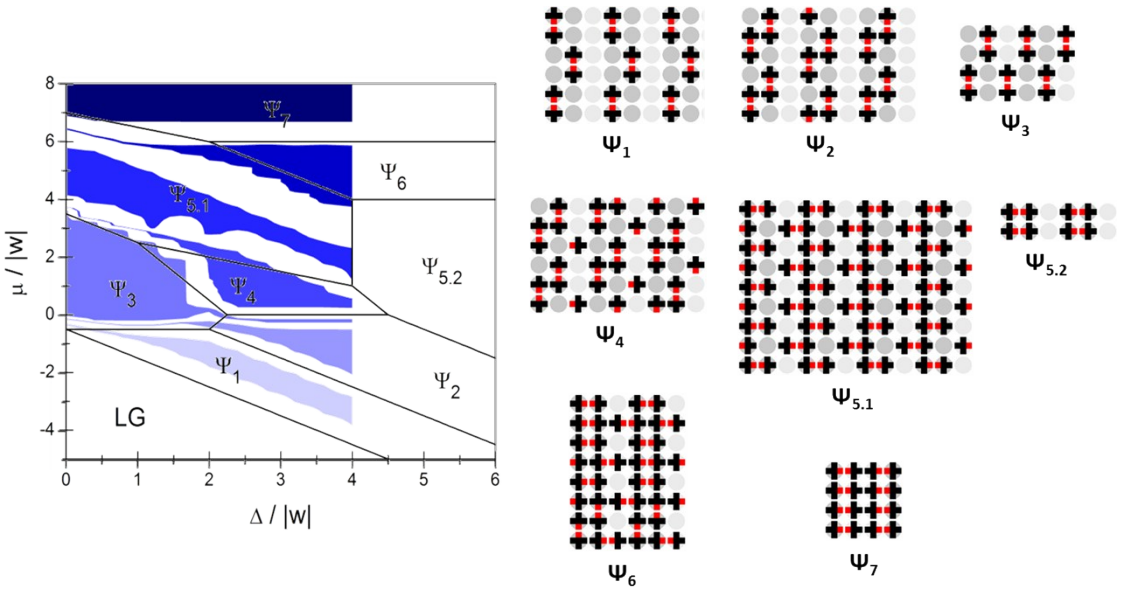
Relation between the notations in the main text of the article and ESI:
LG = LG, D = Ψ_1, L = Ψ_2, D-Ch = Ψ_3, Ch = Ψ_4, Z = Ψ_5, CP = Ψ_6.

Fig. S5 Phase diagram of the adsorption overlayer for the surface with $L_s=1$ and $L_w=2$ topography (left side). Lines are for the ground state phase diagram of the adlayer, and color map corresponds to the regions of the parameter space, where the shown ordered structures had been found with Monte Carlo method at RT/|w|=0.1662. Right side of the figure: the corresponding ordered structures.



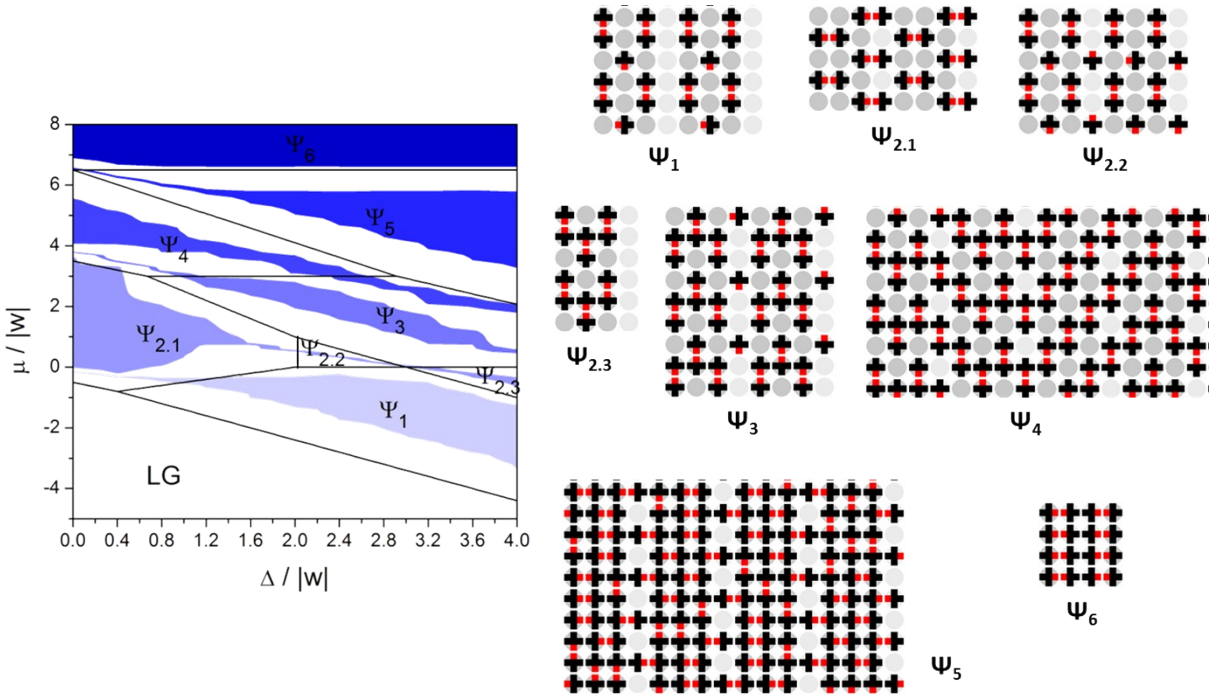
Relation between the notations in the main text of the article and ESI:
LG = LG, D = Ψ_1, L = Ψ_2, Ch = $\Psi_{3.1}$, L-Ch = $\Psi_{3.2}$, Z-Ch = Ψ_4, Z = Ψ_5, CP = Ψ_6.

Fig. S6 Phase diagram of the adsorption overlayer for the surface with $L_s=1$ and $L_w=3$ topography (left side). Lines are for the ground state phase diagram of the adlayer, and color map corresponds to the regions of the parameter space, where the shown ordered structures had been found with Monte Carlo method at RT/|w|=0.1662. Right side of the figure: the corresponding ordered structures.



Relation between the notations in the main text of the article and ESI:
LG = LG, L-Ch = Ψ_1, L-Z = Ψ_2, Ch = Ψ_3, L-Z-Ch = Ψ_4, Z = $\Psi_{5.1}$, L-CP = $\Psi_{5.2}$, L-2DPN = Ψ_6, CP = Ψ_7.

Fig. S7 Phase diagram of the adsorption overlayer for the surface with L_s=*2* and L_w=*1* topography (left side). Lines are for the ground state phase diagram of the adlayer, and color map corresponds to the regions of the parameter space, where the shown ordered structures had been found with Monte Carlo method at RT/|w|=0.1662. Right side of the figure: the corresponding ordered structures.



Relation between the notations in the main text of the article and ESI:
LG = LG, L-D-Ch = Ψ_1, Ch = $\Psi_{2.1}$, D-Ch = $\Psi_{2.2}$, L-Z = $\Psi_{2.3}$, L-Z-Ch = Ψ_3, Z = Ψ_4, L-2DPN = Ψ_5, CP = Ψ_6.

Fig. S8 Phase diagram of the adsorption overlayer for the surface with L_s=*3* and L_w=*1* topography (left side). Lines are for the ground state phase diagram of the adlayer, and color map corresponds to the regions of the parameter space, where the shown ordered structures had been found with Monte Carlo method at RT/|w|=0.1662. Right side of the figure: the corresponding ordered structures.