

PRISM: a phase-resolved surface equation of state enabling automated analysis of Langmuir isotherms

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The interpretation of π -A isotherms of Langmuir monolayers is traditionally limited by subjective manual segmentation and a lack of thermodynamic consistency, particularly within complex phase coexistence regions [1, 2]. Here, we propose the Phase-Resolved Interfacial Surface Model (PRISM), an equation-of-state framework that enables the automated extraction of physically meaningful parameters—structural, mechanical and thermodynamic properties—while ensuring rigorous uncertainty quantification through statistical model selection.

The model is based on fundamental thermodynamic relations for monocomponent monolayers of insoluble surfactants. PRISM integrates domain-correction mechanisms to account for deviations from ideality, such as the sloped coexistence segments often observed experimentally, which arise from phase domain formation and line tension. A nested-model selection strategy activates these corrections only when statistically justified, providing a continuous and thermodynamically consistent description of the isotherm while reducing artifacts associated with conventional analysis.

From π -A isotherms, whether obtained experimentally or from molecular dynamics simulations, PRISM enables the estimation of key structural (e.g.: area per molecule), mechanical (e.g.: compressibility modulus) and thermodynamic quantities (e.g.: changes in chemical potential, Gibbs free energy variations) associated with phase transitions. The model is validated across representative lipid monolayers, providing a consistent and reproducible framework for interfacial thermodynamic characterization.

Keywords:

Langmuir monolayers, interfacial thermodynamics, surface tension, equation of state, phase coexistence, compressibility modulus.

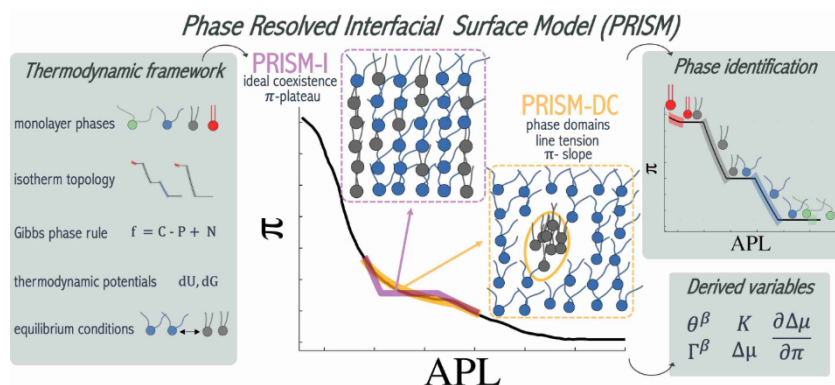


Figure 1: Scheme of the PRISM model proposed as equation of state for π -APL isotherms.

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