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REVIEW about the dissertation thesis "Theoretical modeling of monolayer formation of nonionic surfactants at the air/water interface. Quantum chemical approach" by Elena S. Kartashynska submitted for doctoral degree on specialty 02.00.04 – physical chemistry

Although Langmuir monolayers are not directly relevant for applications in our days, they have gained increasing importance as very useful and easy-to-handle model systems to understand basic problems on a molecular level in life and material sciences. The development of numerous sophisticated highly surface-sensitive techniques led to a drastic increase in experimental investigations of thin amphiphilic films at the liquid-air interface and therefore scientific publications during the last years. Theoretical modeling, which is now possible on a higher level due to the access to extremely powerful computers, is of utmost importance for a better understanding of the properties of such films. The submitted thesis is exactly in the focus of his hot area of science. It is a complex research devoted to the study of thermodynamics and structural parameters of monolayer formation of nonionic surfactants at the air/water interface using quantum chemical semi-empiric PM3 method.

The proposed model allows the access to important monolayer parameters in a reasonable time. Such parameters as the threshold chain length of surfactants for the formation of stable monolayers and geometric parameters of the monolayer unit cell, which can be only measured in time-consuming synchrotron experiments, are of great significance for the film research. The thesis contains very interesting results, which have been published in highly-cited international journals, concerning the relationship between the electronic structure of the surfactant and its threshold chain length. Its value is determined by electron-donor and electron-seeking properties of the surfactant functional groups.

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The other results presented in the paper concern the temperature dependence of monolayer morphology: the temperature increase or equivalent shortening of the hydrocarbon chain length of surfactants result in the increase of content of infinite 'linear' 1D clusters (dendritic growth). One important predictive value of the used approach is the molecular tilt angle of the surfactant with respect to the normal to the interface using the size of the hydrophilic 'head'. This value can be directly compared with experimental data using grazing incidence x-ray diffraction at synchrotron sources.

The publication list, based on the described results, is impressive. 16 of these publications are indexed in WOS, Scopus.

To conclude, the thesis by Elena S. Kartashynska is a fundamental research of outstanding quality. It is devoted to the description of relationships between the surfactant structure and the corresponding thermodynamical and morphological parameters of monolayers formed at the air-liquid interface. The presented work conforms to all standards (actuality, scientific novelty, practical value, high theoretical level and content) qualifying it as a doctoral thesis on the specialty 02.00.04 – physical chemistry. Therefore, I support strongly the author of the thesis Elena S. Kartashynska as highly eligible for the doctoral degree in chemical sciences.

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