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Molecular models of the hair surface

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We introduce a new coarse-grained molecular model of the outer layers of the human hair surface. Chemical damage is captured by means of random removal of grafted lipids. A broad range of degrees of damage is considered. Nanoscale droplet wetting is further evaluated against existing experimental data. The new model is intended to be applied in future nanoscale friction simulations in dry and wet hair-hair contacts.

Keywords: hair surface, grafted monolayers, coarse-grained models, contact angle

1. Introduction

A detailed understanding of the chemical composition and structure of the surface of human hair is important for the development of more effective and sustainable hair care products [1]. The surface of hair is of particular interest since adsorption of formulation components, as well as lubrication between hair fibres, will largely depend on its characteristics [1]. Experimental surface characterization studies of virgin and damaged human hair have shown that compared to virgin hair, damaged hair usually displays increased surface charge density, hydrophilicity, and friction. These effects can be attributed to removal of a 18-MEA fatty acid monolayer and formation of cysteic acid (sulfonate) groups on the surface [2,3]. Atomistic molecular dynamics (MD) simulations of this intact fatty acid layer have been conducted by Cheong et al. [4] to predict the separation distance between fatty acid chains. In the proposed work, we further extend this to a coarse-grained model of the hair surface to study different degrees of chemical damage on the hair surface representative of light bleaching.

2. Methods

The MARTINI 2.0 CG force field [5] is used to derive a coarse-grained representation of the 18-MEA monolayer on the healthy hair cuticles. An excerpt of the model framework is shown in Fig. 1. Chemical damage is represented by randomly removing lipid chains and replacing them by an exposed cysteic acid group. Fully-functionalized and fully damaged monolayers, as well as five intermediate degrees of damage are considered.

3. Results

Thickness and tilt angle statistics are extracted for the new model surfaces and are compared at different grafting distances and degrees of functionalization in a vacuum environment. Furthermore, water and *n*-hexadecane nanodroplets are introduced on the surfaces to study the wetting behavior of polar and non-polar fluids. Consistent with experiments, the model is able to capture the transition from a hydrophobic and oleophilic state towards a hydrophilic/oleophobic wetting behavior. This study paves way for future work to study the adsorption and friction behavior of dry and wet hair contacts at different degrees of damage.

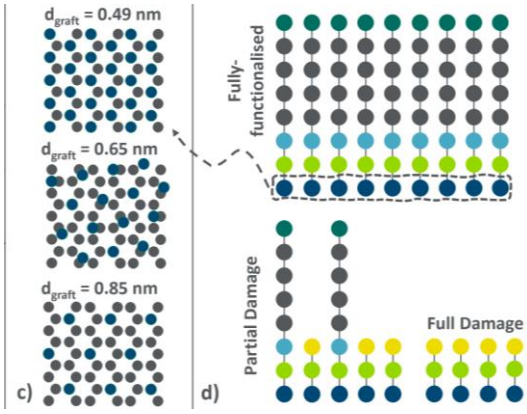

Figure 1: Excerpt of the proposed coarse-grained hair surface model framework using the MARTINI force field [5].

4. References

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