

Hair Keratin Molecular Dynamics Studies

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The keratin is a key element of the hair, nails and skin in vertebrates. Understand the keratin features such as its assembling in the mentioned structures, its interaction with some compounds or mechanical properties is of great interest in the fight against some diseases or in the development and optimization of cosmetic products.

Although molecular dynamics simulations provides unique information at molecular level there are only a few studies using this technique on the study of keratin. This is likely the result of the non-existence of full length keratin crystallographic model. In the few works published about keratin using molecular dynamics simulations the authors had to design and build the computational keratin model, to make the simulations of interest.

This work addresses some molecular dynamics studies about hair keratin, from the physicochemical properties of the molecular models to the correlation of the simulations results with experimental data.

Our work on this field, with recently developed computational models of hair fibers, is also discussed. We built molecular dynamics models able to reproduce in simulations some phenomena observed in experimental assays, providing important information at molecular level about the mechanisms that lead to the experimental results.