Direct calculation of surface free energy of mannitol by Molecular Dynamics simulations

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Surface Free Energy (SFE) is an important property of solid materials in numerous industrial applications ranging from nucleation [1] to powder flowability [2]. The calculation of this quantity through Molecular Dynamics simulations therefore becomes essential, since it allows to obtain the value of the SFE directly from its thermodynamic definition. Among the different methods developed to determine this quantity from computer simulations, the cleaving method [3] calculates the SFE directly in the reversible process that creates a surface (or an interface) from the bulk system while measuring the work done on the system during this process. In this work we show the extension of the cleaving method to a molecular system, the mannitol, which represents a first step towards the development of a multi-scale methodology which will make use of the cleaving method with coarse-graining to obtain the SFE for more complicated systems such as polymers.

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