

The free-energy profile of a fullerene molecule crossing a bio-membrane

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Fullerenes are a variety of molecules composed of carbons. The buckminsterfullerene, also known as buckyball is the most famous component of this family of molecules. It is also the most common in terms of natural occurrence, as it can often be found in soot. The biological importance of this molecule has been studied in the last few years, indicating that this molecule can interact with some proteins, enzymes and molecules inside the cell. For this, the buckyball needs to cross the biological membrane, which is very complicated since this lipid bilayer presents the largest energetic barrier to molecules that require a media exchange.

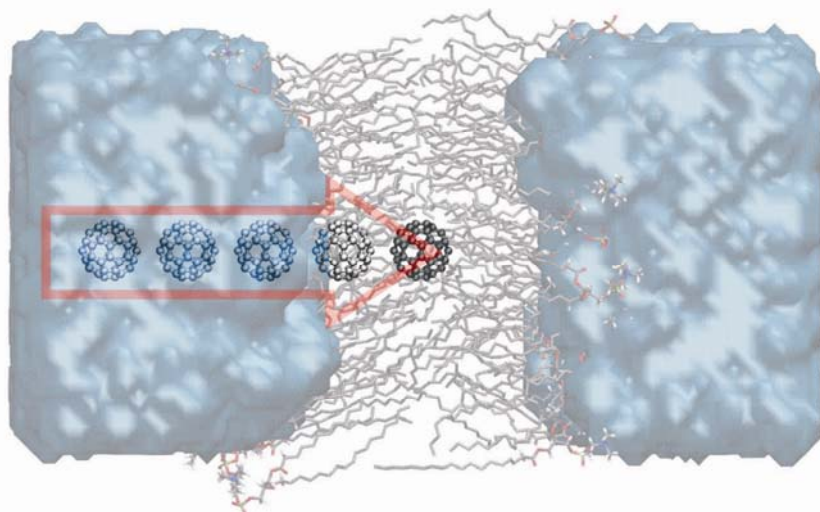


Figure 1: Interaction of fullerene with stearyl-2-oleoylphosphatidylcholine (SOPC) membrane.

We use molecular dynamics methods near equilibrium, in particular the Adaptive Biasing Force (ABF) method, from which we determine the free energy profile for a buckminsterfullerene (C_{60}) molecule in the water / bio-membrane interface. These studies have important potential technological applications, such as drug delivery and side effects of fullerenes on the human cell.

References

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