How to Use Computer Modelling to Complement Experiments

(What you always wanted to know about modelling but you were afraid to ask!)

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Computer modelling has become a fundamental tool to understand and rationalize new nanomaterials, and there is an increasing volume of research that is purely computational. Through the years, we have applied and developed computational models to complement several experimental problems on carbon-based nanomaterials.

We will discuss, **from the experimental point of view** and in a **non-technical manner**, different results of state of the art computer modelling and explain how complex is to perform these simulations. This will be illustrated by several of our computational studies complementing experimental observations of different materials such as carbon nanotubes [1], graphene [2], and molecular crystals [3]. More philosophically, we will try to show you why we believe **most experimental young researchers should also do modelling**.

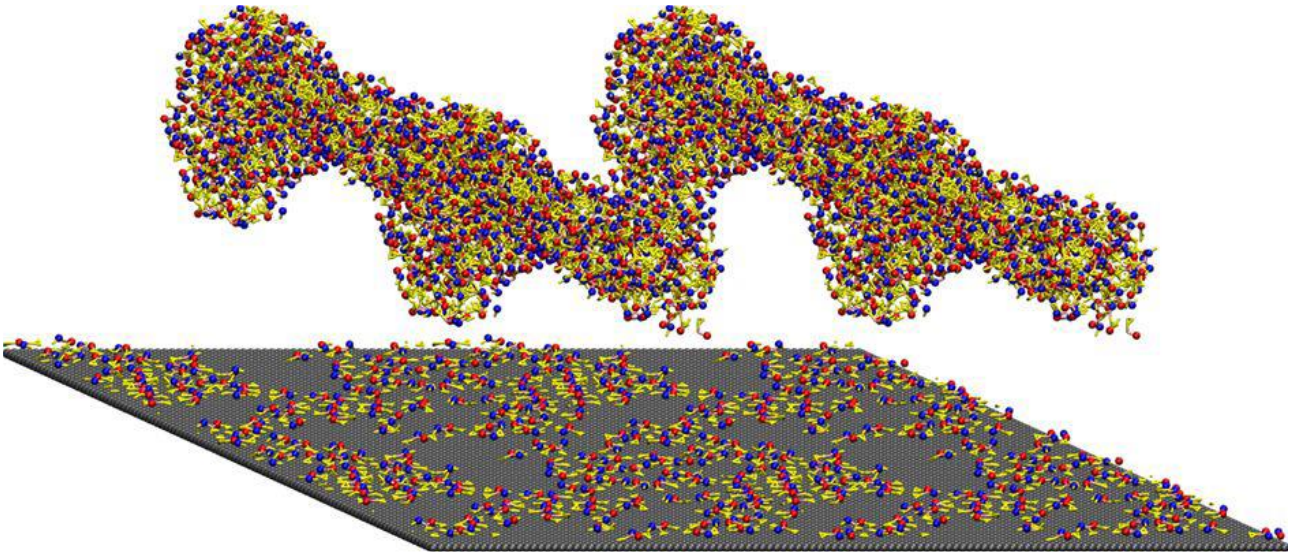

Figure 1. Model of a peptide gel in water on a graphene surface [1].

References

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