# CALCULATION OF NONCONTACT FORCES BETWEEN TITANIA NANOSPHERES: MD STUDIES

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## ABSTRACT

The mechanical properties of polymers could be modified by adding fillers. This combination of a polymer with a filler is called a microcomposite. It was found by Selvin *et al.*[1] that the mechanical properties of titanium dioxide-filled polystyrene microcomposites, such as Young's modulus, tensile strength, elongation at break, flexural modulus and flexural strength, increase linearly with the increase of filler concentration followed by a decrease beyond 15 wt.%. This clearly shows that titanium dioxide reinforces polystyrene matrix effectively at lower filler content. The decrease at higher loading is due to the particle–particle interaction of the titanium dioxide leading to agglomeration.

In order to understand the interaction between the nanoparticles that leads to agglomeration, it is vital to understanding the dynamic behaviors and interrelated aspects between the nanoparticles. In this study, molecular dynamics (MD) simulation will be used to calculate the interaction forces and potentials such as van der Waals attraction, Born repulsion, electrostatic interaction between two titania nanospheres. The results will be compared to those predicted by the adapted continuum models (Hamaker model[2] or Hertz model[3]) to develop the revised formulae to determine the van der Waals attraction and Born repulsion, respectively. Furthermore, the Coulomb's law will be tested for validation in determining the electrostatic potential between nanospheres.

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**Reference:**

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