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21. 25. OUTUBRO • CAMPUS DO VALE

<b>Evento</b>	Salão UFRGS 2019: SIC - XXXI SALÃO DE INICIAÇÃO CIENTÍFICA DA UFRGS
<b>Ano</b>	2019
<b>Local</b>	Campus do Vale - UFRGS
<b>Título</b>	Diagrama de fase de uma mistura Lennard-Jones com interação repulsiva entre solvente e soluto
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Phase diagram of a Lennard-Jones mixture with repulsive interaction between solvent and  
solute

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In molecular dynamics simulations the equation of motion for each particle in the fluid is integrated in order to understand the system's behavior. In these simulations, the Lennard-Jones potential is widely used.

In this research project we performed molecular dynamics simulations in the canonical ensemble (NVT) using the Lennard-Jones potential. We found the pressure versus temperature diagram for a binary mixture in which the repulsion between particles of different species is stronger than for the same species.

This model is useful to understand the dynamics of solvents interacting repulsively with solutes such as a mixture of water and apolar compounds.