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The basis of the MD technique is little more than the integration of the Newton's equation of motion: $F = ma$, to calculate the positions of the atoms over time. The behavior of the atoms in such a calculation can be likened to the movement of billiard balls (Leach, 2001). Of course, billiard balls move in straight lines until they collide with each other and the collisions change their direction ...

The Basic Concepts of Molecular Modeling - ScienceDirect

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Abiogenesis - Wikipedia

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